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Runge-Kutta Schemes for Numerical Discretization of Bilevel Optimal Control Problems

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RUNGE-KUTTA SCHEMES FOR NUMERICAL DISCRETIZATION OF BILEVEL OPTIMAL CONTROL PROBLEMS

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Abstract. In this paper we consider the discretization of bilevel optimal control problems by s-stage Runge-Kutta schemes. Bilevel optimal control problem belong to the class of dynamic or differential games as they are the time-dependent counterpart of finite bilevel optimization problems. The analysis of the Runge–Kutta schemes presented in this paper is based on the continuous optimality system which is derived by replacing the lower-and upper-level control problems, respectively, by their associated necessary optimality conditions . We apply the results of [13, 4, 15] for standard and IMEX Runge-Kutta schemes for general optimal control problems in order to relate the discretization schemes obtained through finite dimensional optimality theory to time-discretizations of the continuous optimality system. Moreover, order conditions up to order three are proven. Finally, we briefly discuss suitable extensions to general leader-follower games.

Keywords. Runge-Kutta schemes, optimal control, bilevel program, hierarchical optimal control, game theory
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1. Introduction. Dynamic Nash games have been considered since the early stages of game theory, see for example the work from A. Bensoussans [3] or J. Cruz [6]. They have applications in various fields such as [12, 17, 19, 20, 25]. See also the recent books [2, 8, 11] on dynamic or differential games, respectively.

In contrast to classical Nash games [26], where all players are at the same level and make their decision simultaneously, bilevel optimization problems model so-called Stackeberg games [34] or single-leader-follower games, i.e. the case of hierarchy among the players of a game in the sense that they split into two groups, so-called leaders and followers. They model the situation of one leader and in general several followers in contrast to so-called multi-leader-follower games, where several leaders and followers exist. The upper-level player (called the leader) makes his decision first and then in a second step, the lower-level players (called the followers) play a Nash-game among each other which is parameterized by the leader's strategy. In this paper, we will focus on two-player games, i.e. single-leader-single-follower games. Moreover, instead of the finite dimensional (i.e. static) game we consider dynamic (time-dependent) game, where each player has an objective functional and as decision variable a control function $u(t)$ or $v(t)$,respectively. However, since the right-hand side of the state equation depends on both strategies, this holds also true for both objective functionals. In the game theoretic context, the terminology bilevel optimal control problem reflects the fact that in the mathematical description of the game, the upper-level (i.e. the leader's) optimal control problem is contrained by the lower-level (i.e. the follower's) optimal control problem. In an inverse programming setting, the upper-level control function can be seen as the design variable that appears as a parameter in the optimal control problem in the lower level [24].

A classical approach to solve bilevel optimization problems is to replace the lower-level problem by the associated optimality conditions, which then yields a single-level problem [1, 7]. The same can be done for the bilevel optimal control problem by applying the Pontryagin maximum principle [**?**, 22]. If the resulting single-level problem is again replaced by its optimality conditions, a system of state and so-called adjoint equations is obtained.

Recently, Runge-Kutta methods for the time discretization of optimal control problems involving differential equations have been discussed in the context of optimal control in various papers [13, 4, 9, 10]. In particular, their properties have been investigated, as follows. In a

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paper by Hager [13] order conditions (up to order four) for Runge–Kutta methods applied to optimality systems are derived. This work has been further extended in [4, 9, 10]. Bonnans et al. [4] and Chyba et al [5] analyse furthermore the properties of symplecticity in the context of optimal control. Further studies of discretizations of state and control constrained problems using Runge–Kutta methods have been presented in [9, 10]. Moreover, in [15] the properties of IMEX Runge–Kutta schemes have been discussed in the context of optimal control problems. In this special class of additive Runge-Kutta methods an implicit RK-discretization is combined with an explicit method (thus the terminology (IMEX)), to resolve stiff and non–stiff dynamics accordingly. These methods have e.g. been studied in [29, 28, 15].

In the present work, we will make use of the results of Hager [13] and Bonnans et al [4] for the standard Runge–Kutta method and the results of [15] for an additive Runge-Kutta scheme applied to the state equation. We are interested in the relations of the discretization of the optimality systems and the corresponding order conditions of the resulting scheme.

The paper is organized as follows. In Section 2, we will first introduce the bilevel optimal control problem. Then we will stepwise derive the continuous necessary optimality system for the bilevel optimal control problem using the Pontryagin maximum principle [22] first for the lower-level control problem and then for the resulting single-level problem for the upper-level control. Next, in Section 3 we introduce the s-stage Runge–Kutta discretization of the state equation and similar to the procedure in Section 2, we stepwise derive the discrete system of necessary optimality conditions by applying the KKT conditions first to the lower-level problem and then to the obtained discrete single-level problem for the (discrete) upper-level variable. We compare the obtained system to a Runge–Kutta time discretization of the continuous optimality system we derived in Section 2. The result is summarized in Theorem 3.1. Applying results of Hager and Bonnans et al [13, 4] and Herty et al [15], we prove order conditions for this system up to order three in Section 4. Finally, in Section 5, we give a short overview on further extensions to more general bilevel problems or leader-follower-games, respectively.

2. The optimal control problem. We consider the bilevel optimal control problem of the type (2.1):

$$
\begin{aligned}
(BOCP) \qquad & \min_{v,u,x} \quad J(x(T)) \\
& \quad \text{s.t.} \quad \min_{u,x} j(x(T)) \\
& \qquad\qquad \text{s.t. } \dot{x}(t) = f(x(t),u(t),v(t)), \qquad t \in [0,T] \\
& \qquad\qquad\quad x(0) = x^0 \qquad ,
\end{aligned}
\tag{2.1}
$$

where we assume that the objective functionals J and j and the right-hand side $f(x,u,v)$ are sufficiently smooth.

These kind of optimal control problems belong to the class of hierarchical control problem, where the so-called upper-level control problem is constrained by another, the so-called lower-level problem, i.e. the upper-level objective functional has to be minimized subject to the fact that u and x solve the lower-level problem that is given by

$$
\begin{aligned}
(LLCP) \qquad & \min_{u,x} j(x(T)) \\
& \quad \text{s.t. } \dot{x}(t) = f(x(t),u(t),v(t)), \qquad t \in [0,T] \\
& \qquad x(0) = x^0 \qquad .
\end{aligned}
\tag{2.2}
$$

Associated with this lower-level optimal control problem we define the lower-level Hamiltonian function $\check{H}$ as [22]

$$\check{H}(x,v,u,\lambda) := \lambda^T f(x,u,v),$$

where λ is the so-called adjoint of the lower-level control problem. Under appropriate conditions it is well–known [16, 22, 33] by the Pontryagin maximum principle [22] that the first–order necessary optimality conditions for the lower-level problem of (2.1) are given by

$$\dot{x} = \quad D_\lambda \check{H}(x, v, u, \lambda) = f(x, u, v), \qquad x(0) = x^0 \tag{2.3a}$$

$$\dot{\lambda} = -D_x \check{H}(x, v, u, \lambda) = -f_x(x, u, v)^T \lambda, \qquad \lambda(T) = j'(x(T)) \tag{2.3b}$$

$$0 = \quad D_u \check{H}(x, v, u, \lambda) = -f_u(x, u, v)^T \lambda. \tag{2.3c}$$

Equation (2.3a) is called state equation whereas (2.3b) is called the adjoint equation associated with (2.1). Now, replace the optimal control problem (2.2) in the constraints of (2.1) by the optimality conditions (2.3). This yields a single-level optimal control problem and corresponds to an approach similar to what is often done for finite-dimensional (i.e. static) bilevel optimization problems, where it results in so-called mathematical programs with equilibrium or complementarity constraints, respectively (depending on whether the optimality conditions of the lower-level problem are given in terms of a variational inequality or the KKT conditions that generally involve complementarity conditions). The single-level optimal control problem resulting for (BOCP) is

$$(SOCP^0) \qquad \begin{array}{lll} \min_{v,u,x,\lambda} & J(x(T)) & \\ \text{s.t.} \quad \dot{x} & = f(x, u, v), & x(0) = x^0 \\ \quad\;\; \dot{\lambda} & = -f_x(x, u, v)^T \lambda, & \lambda(T) = j'(x(T)) \\ \quad\;\; 0 & = -f_u(x, u, v)^T \lambda. & \end{array} \tag{2.4}$$

Now, as in e.g. [4, 13, 15], we suppose that u is implicitly given by (2.3c), i.e. we assume that there exist a continuously differentiable function $\theta(v, x, \lambda)$ so that, given v, x and λ, $u(t) = \theta(v(t), x(t), \lambda(t))$ satisfies (2.3c). In that case, we can then reduce (2.4) to

$$(SOCP) \qquad \begin{array}{lll} \min_{v,\lambda,x} & J(x(T)) & \\ \text{s.t.} \quad \dot{x} & = f(x, \theta(v, x, \lambda), v), & x(0) = x^0 \\ \quad\;\; \dot{\lambda} & = -f_x(x, \theta(v, x, \lambda), v)^T \lambda, & \lambda(T) = j'(x(T)) \end{array} \tag{2.5}$$

Define

$$F(x, v, \lambda) = \begin{pmatrix} f(x, \theta(v, x, \lambda), v) \\ -f_x(x, \theta(v, x, \lambda), v)^T \lambda \end{pmatrix}$$

Next, we proceed with the upper-level problem as we did for the lower-level problem, i.e. we define the upper-level Hamiltonian funtion $\hat{H}$.

$$\hat{H}(x, v, \lambda, p) := p^T F(x, v, \lambda)\,,$$

where $p = (p_x, p_\lambda)^T$ is the adjoint of the upper-level control problem. Hence the first–order optimality conditions of (2.5) are given by

$$\dot{\begin{pmatrix} x \\ \lambda \end{pmatrix}} = \quad D_p \hat{H}(x, v, \lambda, p) = F(x, v, \lambda), \tag{2.6a}$$

$$\dot{p} = -D_{x,\lambda} \hat{H}(x, v, \lambda, p) = -F_{x,\lambda}(x, v, \lambda)^T p, \tag{2.6b}$$

$$0 = \quad D_v \hat{H}(x, v, \lambda, p) = -F_v(x, v, \lambda)^T p. \tag{2.6c}$$

with

$$F_{x,\lambda}(x,v,\lambda) = \begin{pmatrix} f_x + f_u\theta_x & f_u\theta_\lambda \\ -(f_{xx} + f_{xu}\theta_x) & -(f_{xu}\theta_\lambda + f_x) \end{pmatrix}$$

together with the boundary conditions

$$x(0) = x^0, \qquad \lambda(T) = j'(x(T)) \tag{2.7}$$

$$p_x(0) = 1, \qquad p_x(T) = J'(x(T)) \tag{2.8}$$

$$p_\lambda(0) = 0, \qquad p_\lambda(T) = 0\,. \tag{2.9}$$

Notice, that in (2.6) the state equation of the single-level optimal control problem (SOCP) is of the form

$$\dot{\begin{pmatrix} x \\ \lambda \end{pmatrix}} = G^1(x,\lambda,v) + G^2(x,\lambda,v)$$

with the functions G^1 and G^2 being defined as

$$G^1(x,\lambda,v) = \begin{pmatrix} G^{11} \\ G^{12} \end{pmatrix} = \begin{pmatrix} f(x,\theta(v,x,\lambda),v) \\ 0 \end{pmatrix} \tag{2.10}$$

$$G^2(x,\lambda,v) = \begin{pmatrix} G^{21} \\ G^{22} \end{pmatrix} = \begin{pmatrix} 0 \\ -f_x(x,\theta(v,x,\lambda),v)^T\lambda \end{pmatrix}\,. \tag{2.11}$$

Moreover, let $z := (x,\lambda)$, then the problem (SOCP) may be written in a similar form of the optimal control problem that is studied in [15].

$$\begin{array}{rcll} \min_{v,z}\ \tilde{J}(z(T)) & := & J(x(T)) & \\ \text{s.t.} \qquad \dot{z} & = & \varphi(z,v) + \psi(z,v), & \qquad \Phi(z(0),z(T)) = 0 \end{array} \tag{2.12}$$

with $\varphi(z,v) = G^1(x,\lambda,v)$ and $\psi(z,v) = G^2(x,\lambda,v)$. We may thus use the analysis therein, to investigate the problem (SOCP).

3. Runge-Kutta discretizations. We are interested in Runge–Kutta discretizations for the state equation (2.3a) and the resulting discretizations schemes of (2.3b), (2.3) and finally of (2.6). We will thus use results from [4, 13, 15] to analyse the relations between the different levels of discretization. We first start with a Runge–Kutta discretization with s stages applied to the state equations (2.3a). Such a scheme applied to (2.3a) is given by [14]

$$X_n^{(i)} = x_n + h\sum_{j=1}^{s} a_{ij} f(X_n^{(j)}, u_n^j, v_n^j) \qquad i = 1,..,s \tag{3.1a}$$

$$x_{n+1} = x_n + h\sum_{i=1}^{s} \omega_i f(X_n^{(i)}, u_n^i, v_n^i), \qquad n = 0,1,2,. \tag{3.1b}$$

where A,ω are the associated Runge–Kutta coefficient matrix and the Runge–Kutta weights, respectively. We then analyse the resulting schemes that we obtain if we apply standard finite dimensional optimality theory (i.e. setting the derivative of the Lagrangian function equal to zero) first to the lower-level control problem (LLCP) of the bilevel problem (BOCP), where the continuous state equation is discretized by (3.1) and the controls accordingly and secondly to the resulting discrete single-level optimization problem. As we will see, the discretization schemes that we obtain by applying the optimality condtions, belong to the class of partitioned Runge-Kutta schemes applied to the different optimality systems. In Figure 3.1 we summarize our findings. For simplicity reasons, in the following, we will ommit the discretizations of the boundary conditions, as they do not change the outcomes.

Instead of the representation (3.1) one can use an equivalent formulation of this RK scheme, which is given by [14, 4]

$$K_n^{(i)} = f(x_n + h\sum_{j=1}^{s} a_{ij} K^{(j)}, u_n^i, v_n^i) \tag{3.2a}$$

$$x_{n+1} = x_n + h\sum_{i=1}^{s} \omega_i K_n^{(i)}, \tag{3.2b}$$

and used in [4, 15] in order to derive the discrete first–order optimality conditions. The associated discrete bilevel optimization problem according to this discretization becomes

$$
\begin{array}{llll}
(BDOP) & \min_{v,u,x,K} & J(x_N) & \\
 & \text{s.t.} & \min_{u,x,K} \; j(x_N) & \\
 & & \text{s.t.} \; K_n^{(i)} = f(x_n + h\sum_{j=1}^{s} a_{ij} K_n^{(j)}, u_n^i, v_n^i) & i = 1,..s \\
 & & & n = 0,1,2,..,N-1 \\
 & & \quad x_{n+1} = x_n + h\sum_{i=1}^{s} \omega_i f(X_n^{(i)}, u_n^i, v_n^i), & n = 0,1,2,..,N-1 \\
 & & x_0 = x^0. &
\end{array}
\tag{3.3}
$$

In [4, 13] it is shown, that applying the standard finite-dimensional optimality conditions and carry out suitable variable transformations for the associated finite adjoint variables, the RK-discretization (3.1) and (3.2) yield the discrete optimality system

$$X_n^{(i)} = x_n + h\sum_{j=1}^{s} a_{ij} f(X_n^{(j)}, u_n^j, v_n^j) \tag{3.4a}$$

$$x_{n+1} = x_n + h\sum_{i=1}^{s} \omega_i f(X_n^{(i)}, u_n^i, v_n^i), \tag{3.4b}$$

$$\Lambda_n^{(i)} = \lambda_n - h\sum_{j=1}^{s} \tilde{a}_{ij} \, f_x(X_n^{(j)}, u_n^j, v_n^j)^T \Lambda_n^{(j)} \tag{3.4c}$$

$$\lambda_{n+1} = \lambda_n - h\sum_{i=1}^{s} \tilde{\omega}_i \, f_x(X_n^{(i)}, u_n^i, v_n^i)^T \Lambda_n^{(i)}. \tag{3.4d}$$

with $n = 0, 1, .., N-1$ and

$$\tilde{\omega}_i = \omega_i, \qquad \tilde{a}_{ij} = \omega_j - \frac{\omega_j}{\omega_i} a_{ji}, \qquad \forall\, i = 1,2,..,s\,, \quad j = 1,2,..,s \tag{3.5}$$

This discretization scheme corresponds to a partitioned, symplectic RK-scheme for the state and adjoint equation of the lower-level optimality system (2.3) as is proved in [4, 13]. Therefore, if we substitute u_n^i by $\theta(v_n^i, X_n^{(i)}, \Lambda_n^{(i)})$ and replace the lower-level problem of (BDOP) by the reformulated discrete optimality conditions, i.e. by (3.4), then the resulting discrete optimization problem corresponds to a discretization of the continuous single-level problem $(SOCP)$

$$
\begin{aligned}
(SDOP) \qquad \min_{v,u,x,K} \;& J(x_N) \\
\text{s.t.}\;& X_n^{(i)} = x_n + h \textstyle\sum_{j=1}^s a_{ij} f(X_n^{(j)}, u_n^j, v_n^j) \\
& x_{n+1} = x_n + h \textstyle\sum_{i=1}^s \omega_i f(X_n^{(i)}, u_n^i, v_n^i), \\
& \Lambda_n^{(i)} = \lambda_n - h \textstyle\sum_{j=1}^s \tilde{a}_{ij}\, f_x(X_n^{(j)}, u_n^j, v_n^j)^T \Lambda_n^{(j)} \\
& \lambda_{n+1} = \lambda_n - h \textstyle\sum_{i=1}^s \tilde{\omega}_i\, f_x(X_n^{(i)}, u_n^i, v_n^i)^T \Lambda_n^{(i)}.
\end{aligned} \tag{3.6}
$$

Note, that by our discussion in the previous section, this problem correlates with a discretized version of the optimal control problem (SOCP) using a partitioned RK-scheme for the state equations of the variables x and λ. Hence, the analysis and the results of [15] can be applied and the resulting final discrete first–order optimality system corresponds to an additive, symplectic RK-scheme (with 4 schemes, as $\omega = \tilde{\omega}$) for the continuous optimality system (2.6)

$$X_n^{(i)} = x_n + h \sum_{j=1}^s a_{ij} f(X_n^{(j)}, u_n^j, v_n^j), \tag{3.7a}$$

$$x_{n+1} = x_n + h \sum_{i=1}^s \omega_i f(X_n^{(i)}, u_n^i, v_n^i), \tag{3.7b}$$

$$\Lambda_n^{(i)} = \lambda_n - h \sum_{j=1}^s \tilde{a}_{ij}\, f_x(X_n^{(j)}, u_n^j, v_n^j)^T \Lambda_n^{(j)} \tag{3.7c}$$

$$\lambda_{n+1} = \lambda_n - h \sum_{i=1}^s \tilde{\omega}_i\, f_x(X_n^{(i)}, u_n^i, v_n^i)^T \Lambda_n^{(i)}. \tag{3.7d}$$

$$\tilde{P}^{(i)} = p_n - h \sum_{j=1}^s \alpha_{ij}\, G^{11}_{x,\lambda}(X_n^{(j)}, \Lambda_n^{(j)}, v_n^j)^T \tilde{P}^{(j)}, \tag{3.7e}$$

$$P^{(i)} = p_n - h \sum_{j=1}^s \beta_{ij}\; G^{22}_{x,\lambda}(X_n^{(j)}, \Lambda_n^{(j)}, v_n^j)^T P^{(j)}, \tag{3.7f}$$

$$p_{n+1} = p_n - h \sum_{i=1}^s \omega_i\, (G^{11}_{x,\lambda}(X_n^{(i)}, \Lambda_n^{(i)}, v_n^i)^T \tilde{P}^{(i)} + G^{22}_{x,\lambda}(X_n^{(i)}, \Lambda_n^{(i)}, v_n^i)^T P^{(i)}) \tag{3.7g}$$

with $n = 0, 1, .., N-1$, $i = 1, 2, .., s$, the functions G^1 and G^2 as previously defined and the coefficients α_{ij} and β_{ij} given by

$$\alpha_{ij} := \omega_j - \frac{\omega_j}{\tilde{\omega}_i} \tilde{a}_{ji}, \quad \beta_{ij} := \omega_j - \frac{\omega_j}{\omega_i} a_{ji}$$

with $\tilde{a}_{ij}$ as in (3.5).

Remark 3.1. Note that the upper-level adjoint state p partitions in (p_x, p_λ) as do their discrete approximations $\tilde{P}^{(i)}$ and $P^{(i)}$, respectively. Moreover, due to their special structure the derivatives of $G^1(x, \lambda, v)$ and $G^2(x, \lambda, v)$ are of the type $(A\ 0)^T$ and $(0\ B)^T$ such that in contrast to the general case as discussed in [15] the equations (3.7e) and (3.7f) are not of a mixed type.

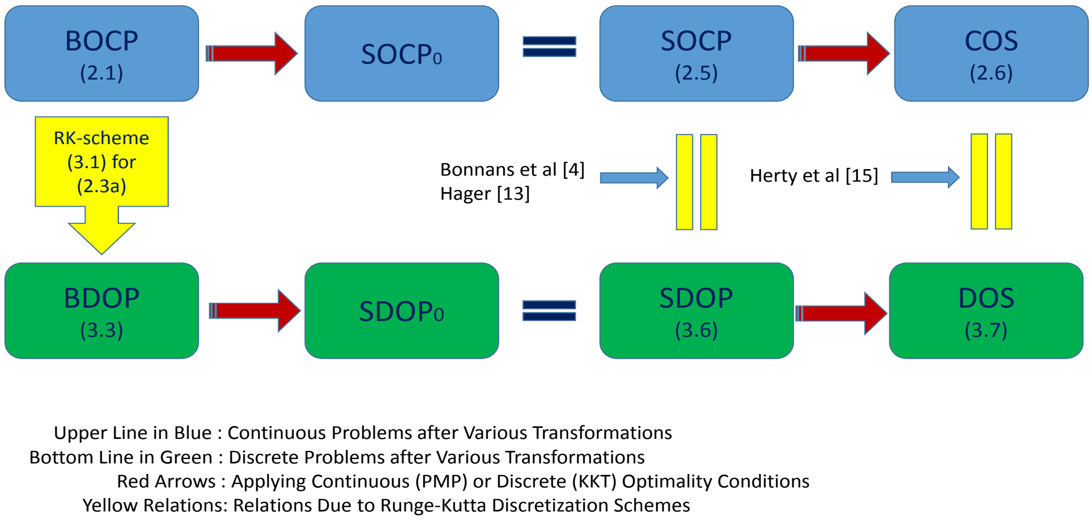

FIG. 3.1. *Diagram summarizing the relations discussed.*

We summarize the previous outcomes in the following Theorem and sketch the interconnections of the various problems in Figure 3.1.

Theorem 3.1. *Consider the problem (2.1) that incorporates the lower-level problem (2.2) whose first–order necessary optimality conditions are given by (2.3). Assume that* $\omega_i \neq 0$ *for all* $i = 1, \dots, s$. *Then,*

1. *replacing the continuous state equation of (2.2) by the RK discretization scheme (3.1) or (3.2), respectively, yields a discrete version of (2.5), where the state equations in the constraints are discretized by a partitioned Runge-Kutta scheme.*
2. *the associated discrete first–order optimality system for (3.6) is given by (3.7). Furthermore, let* $z_n = (x_n, \lambda_n)$ *and* $Z_n^{(i)} = (X_n^{(i)}, \Lambda_n^{(i)})$ *and denote by* $\varphi^{(i)} := \varphi(Z_n^{(i)}, v_n^i)$ *and* $\psi^{(i)} := \psi(Z_n^{(i)}, v_n^i)$ *(cf. (2.12)). Then the system (3.7) form an additive RK discretization of (2.6), provided that for the discretization of (2.6c) we use*

$$\hat{H}^h(z_n, p_{n+1}, v_n) := p_{n+1}^T \left[\sum_{i=1}^{s} (\omega_i \varphi^{(i)} + \omega_i \psi^{(i)}) \right]. \tag{3.8}$$

4. Order conditions Runge-Kutta discretizations. In the following, we will discuss the theoretical properties of the RK-discretization scheme (3.7). In particular we will use the results of Kennedy and Carpenter [18] and Herty et al. [15] in order to analyse the order conditions. First, we give a result concerning the order of the RK-discretization scheme for (3.4). Define the coefficients

$$c_i = \sum_{j=1}^{s} a_{ij}, \qquad \tilde{c}_i = \sum_{j=1}^{s} \tilde{a}_{ij},$$

and

$$d_j = \sum_{i=1}^{s} \omega_i \, a_{ij}, \qquad \tilde{d}_j = \sum_{i=1}^{s} \omega_i \, \tilde{a}_{ij} \, .$$

Then, applying Theorem 4.1 of Hager [13] we obtain the following result.

Theorem 4.1. *Consider the partitioned Runge-Kutta method (3.1) together with (3.4) as a discretization scheme for (2.3). Then the following results hold true.*

1. *The partitioned RK method is of first order, if the RK method (3.1) is of first order.*
2. *The partitioned RK method is of second order, if the RK method (3.1) is of second order.*
3. *The partitioned RK method is of third order, if the RK method (3.1) is of third and it additionally satisfies*

$$\sum_{i=1}^{s} \frac{d_i^2}{\omega_i} = \frac{1}{3} \, . \tag{4.1}$$

Next, we use Theorem 3.1 of Herty et al [15] in order to prove an order result for the additive RK-discretization (3.7) of the optimality system (2.6).

Theorem 4.2. *Consider the additive Runge-Kutta method (3.7) as a discretization scheme for (2.6). Then the following results hold true.*

1. *The additive RK method is of first order, if the RK method (3.1) is of first order.*
2. *The additive RK method is of second order, if the RK method (3.1) is of second order.*
3. *The additive RK method is of third order, if the RK method (3.1) is of third order and additionally satisfies (4.1).*

Proof. Applying Theorem 3.1 of Herty et al [15] and Theorem 4.1, we directly obtain the the first and second order of our additive RK scheme (3.7).

For the third order property, however, we need to prove, that the conditions

$$\sum_{i=1}^{s} \frac{\tilde{d}_i^2}{\omega_i} = \frac{1}{3} \qquad \text{and} \qquad \sum_{i=1}^{s} \frac{d_i \, \tilde{d}_i}{\omega_i} = \frac{1}{3} \tag{4.2}$$

are satisfied. Hence, consider first

$$\begin{aligned} \tilde{d}_i &= \sum_{j=1}^{s} \omega_j \tilde{a}_{ji} \qquad (4.3) \\ &= \sum_{j=1}^{s} \omega_j (\omega_i - \frac{\omega_i}{\omega_j} a_{ij}) = \omega_i \, (1 - c_i) \, . \end{aligned}$$

Hence,

$$\begin{aligned} \sum_{i=1}^{s} \frac{\tilde{d}_i^2}{\omega_i} &= \sum_{i=1}^{s} \frac{\omega_i^2}{\omega_i} (1 - c_i)^2 \\ &= \sum_{i=1}^{s} \omega_i^2 (1 - 2c_i + c_i^2) = \frac{1}{3} \, . \end{aligned}$$

And moreover,

$$\sum_{i=1}^{s} \frac{d_i\,\tilde{d}_i}{\omega_i} = \sum_{i=1}^{s} d_i(1-c_i) = \frac{1}{3}\,.$$

In Table 4.1 we display the third order RK scheme that has been proposed by Hager [13] which has three stages and satisfies the additional condition (4.1).

$$(A,\omega):\quad \begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 1 & -1 & 2 & 0 \\ \hline & 1/6 & 2/3 & 1/6 \end{array} \qquad (\tilde{A},\tilde{\omega}):\quad \begin{array}{c|ccc} 0 & 1/6 & -4/3 & 7/6 \\ 1/2 & 1/6 & 2/3 & -1/3 \\ 1 & 1/6 & 2/3 & 1/6 \\ \hline & 1/6 & 2/3 & 1/6 \end{array}$$

TABLE 4.1

HAG(3,3,3) corresponds to the third-order scheme proposed by Hager in [13] and $(\tilde{A},\tilde{\omega})$ refers to the associated scheme for the adjoint equations of the lower-level problem that satisfies (3.5).

5. Extensions to General Dynamic Leader-Follower Games. So far, we have only investigated the simple bilevel optimal control problem 2.1, where next to the state equation in the lower level, no further constraints appear. In this section, we will give a brief outlook on bilevel control problems, that are more general in the sense that incorporate inequality contraints on the upper-level or lower-level control funtion $v(t)$ or $u(t)$, respectively or consider games with more that two players.

We first start our discussion with convex control constraints $v \in V$ on the upper level only, i.e. we consider

$$\begin{array}{llll} (BOCP_c) & \min_{v,u,x} & J(x(T)) & \\ & \text{s.t.} & \min_{u,x}\ j(x(T)) & \\ & & \quad \text{s.t. } \dot{x}(t) = f(x(t),u(t),v(t)), & t \in [0,T] \\ & & \quad x(0) = x^0 & \\ & & \quad v(t) \in V & a.e. \quad t \in [0,T] \end{array}$$

with some closed, convex set $V \subset \mathbb{R}^n$. In that case, the first part of the approach in Section 2 can be done analoguously and we obtain a single-level optimal control problem similar to (2.5). However, in the next step, we have to take care of the additional constraints on the upper level, which then yield the variational inequality: find $v \in V$ such that

$$D_v\hat{H}(x,v,\lambda,p)^T(w-v) \geq 0 \qquad \text{for all} \qquad w \in V \tag{5.1}$$

instead of the equality $D_v\hat{H}(x,v,\lambda,p) = 0$ in (2.6) [13]. Here, the resulting optimality conditions are therefore also referred to as a differential variational inequality [27]. In [31], it is shown that if the state equation is discretized using an s-stage Runge–Kutta scheme, under suitable conditions, the associated state and control approximations will converge to a solution of the problem. In addition to that, in that case a similar analysis, as is done for standard s-stage Runge–Kutta schemes in [13], has then to be investigated for additive or partitioned Runge–Kutta schemes (since the state equation of the associated single-level optimal control problem is discretized by a partitioned Runge–Kutta scheme).

In the case that we have control constraints in the lower-level control problem, we obtain a dynamic (time-dependent) version of a mathematical program with complementarity constraints

(MPCC) (cf. e.g. [22]). Since these do already pose serious difficulties in the finite-dimensional setting [23, 21, 32, 30] due to their nonconvex, nonsmooth and combinatorial structure and must therefore theoretically as well as numerically be addressed with special care, these problems have to be analysed seperately.

Finally, dynamic Stackelberg games and dynamic multi-leader-follower games can also be adressed similarly to what has been presented in this paper. However, if the optimal control problems are replaced by their necessary optimality conditions, one will essentially find Nash stationary points rather than Nash equilibria. Furthermore, replacing the optimal control problem of each player by its optimality conditions yields a very large optimality system. In this paper, we therefore decided to discuss the two-player leader-follower game and discuss the more complex game models in a seperate paper.

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