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High order variational numerical schemes with application to Nash - MFG vaccination games

Laetitia LAGUZET

ABSTRACT.

This paper introduces high-order explicit Runge-Kutta numerical schemes in metric spaces. We show that our approach reduces to corresponding Runge-Kutta schemes if the ambient space is Hilbert.

We apply these schemes to compute the Nash equilibrium in a Mean Field vaccination Game. Numerical simulations show improvement in the speed of convergence towards the Nash equilibrium; the numerical scheme has high order (two to four) in time.

1 State of the art and motivation

The games with a continuum of agents have been widely studied during the last decade thanks to the *Mean Field Games* (MFG) theory, introduced by Lasry-Lions ([16, 17, 18]) and Huang-Caines-Malhamé ([13, 11, 12]). An application of this framework is the modeling of the vaccination decision in a population. In this case, the Nash-MFG equilibrium corresponds to a strategy where nobody has interest to change his own vaccination strategy; therefore the existence and the determination of an equilibrium is central. Analytic solutions are available for some particular cases (see for instance [15]) but finding an equilibrium becomes more complicated if the model has specific behavior with network interaction or epidemic spread for example ([10, 9, 8]). Thus finding the equilibrium can quickly become time consuming. One commonly used method is based on finding a fixed point of some function, which can be formulated as the attractor of an evolution system.

The existence of an equilibrium in the general case of MFG is of utmost interest (see for instance [2, 4] for an entry point to this literature). Several approaches were developed, inspired by the general framework of gradient flows

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(see [14]) where the procedure is iterative. Let us recall that in a gradient flow framework (which is not necessarily related to a MFG model !) the equation to be solved is written symbolically (see [1] for an introduction):

$$\xi'(t) = \nabla F(\xi(t)), \quad (1)$$

where the function F is given but ∇F cannot be computed. The numerical counterpart of (1) is the celebrated JKO (see [14]) scheme which can be written as:

$$\xi(t_{k+1}) \simeq \operatorname{argmin}_{\eta} \frac{d(\xi(t_k), \eta)^2}{2\tau} + F(\eta). \quad (2)$$

Very recently, second order in time methods have been proposed (see [19]).

On the other hand, a MFG equilibrium has no associated function ' F ' and it is likely that no such function exists. Rather, the search for an equilibrium takes the form of a fixed point:

$$\xi(t) = J(\xi(t)). \quad (3)$$

In practice, inspired by the *Fictitious Game* (see [5]) and *Best Reply* (see [4, 3]) procedures, a new algorithm has been introduced in [9, Eq 3.2] and [20] with the following form:

$$\xi_{k+1} \in \operatorname{argmin}_{\eta} \left\{ \frac{d(\eta, \xi_k)^2}{2\tau} + \mathcal{P}(\eta, \xi_k) \right\}. \quad (4)$$

In the limit $\tau \rightarrow 0$ the equation (4) describes a curve which under some assumptions on \mathcal{P} will be called a solution of the evolution equation $\xi'(t) = \mathcal{P}(\cdot, \xi(t))$. On the other hand, the MFG framework provides a natural function $\mathcal{P}(\cdot, \cdot)$ even when ξ does not belong to a Hilbert space but only to a metric space. Thus we are led to consider evolution equations in metric spaces with semi-explicit numerical schemes (see [20] and also [6]). The purpose of this work is to introduce variational Runge-Kutta explicit methods of high order in a metric space using a generalization of linearity (presented in [7]).

These approaches are applied to the control of epidemic spread with voluntary vaccination as in [9].

The paper is structured as follows: Section 2 is dedicated to the Runge-Kutta method recalling its general form (subsection 2.1) and then the introduction of variational Runge-Kutta methods (subsection 2.2). The equivalence of the two approaches in a Hilbert space is proved in subsection 2.3. Then Section 3 gives numerical application of the different schemes and some considerations are discussed in Section 4. Further details concerning the epidemiological model used in numerical application are provided in Appendix A.

2 Runge-Kutta methods

2.1 In a Hilbert space

Let \mathcal{H} be a Hilbert space, $f : [0, T] \times \mathcal{H} \rightarrow \mathcal{H}$ a regular function and $y : [0, T] \rightarrow \mathcal{H}$ satisfying (in some sense to be specified):

$$y'(t) = f(t, y(t)). \quad (5)$$

The Runge-Kutta approach is an iterative method using temporal discretization in order to obtain a numerical solution of an ordinary differential equation of type (5). The time horizon T is supposed to be finite and can be discretized in $(N_T + 1)$ time instants $t_0 = 0, t_1 = \tau, t_2 = 2\tau, \dots, t_{N_T} = T$ where τ is the time step. Let $y_k \in \mathcal{H}$ be an approximation of $y(t_k)$.

Runge-Kutta method is based on the evaluation at intermediate points in time. Equation (6) presents the general form of the Runge-Kutta method for (5).

$$\begin{array}{c|cccc}
 c_1 & a_{1,1} & a_{1,2} & \dots & a_{1,s} \\
 c_2 & a_{2,1} & a_{2,2} & \dots & a_{1,s} \\
 \dots & \dots & \dots & \dots & \dots \\
 \hline
 & b_1 & b_2 & \dots & b_s
 \end{array}
 \quad
 \begin{aligned}
 y_{k+1} &= y_k + \tau \sum_{i=1}^s b_i p_i, \\
 p_i &= f \left(t_n + c_i \tau, y_k + \tau \sum_{j=1}^{i-1} a_{i,j} p_j \right).
 \end{aligned}
 \quad (6)$$

Figure 1: Runge-Kutta method. **Left:** Butcher tableau. **Right:** Equation.

A method is defined by the values of the coefficients b_i , c_i and $a_{i,j}$, often presented in the *Butcher tableau* (see table in figure 1). Consistency of such a method is ensured if $\sum_{j=1}^{i-1} a_{i,j} = c_i$ for $i = 2, \dots, s$.

We will present below some particular schemes that will later be formulated in a metric space.

2.1.1 Explicit Euler scheme

The Explicit Euler (denoting EE) scheme is a Runge-Kutta method with only one step. It is defined in figure 2 by the Butcher tableau or equivalently by equation (7). In this case, this scheme is of order one in time.

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array} \qquad y_{k+1} = y_k + \tau f(t_k, y_k). \quad (7)$$

Figure 2: Explicit Euler method. **Left:** Butcher tableau. **Right:** Equation.

2.1.2 Heun scheme

Heun scheme uses an approximate value p_1 , in order to compute y_{k+1} , see the figure 3. This scheme is of order two in time.

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array} \qquad \begin{array}{l} p_1 = y_k + \tau f(t_k, y_k), \\ y_{k+1} = y_k + \frac{\tau}{2} \left[f(t_k, y_k) + f(t_{k+1}, p_1) \right]. \end{array} \quad (8)$$

Figure 3: Heun method. **Left:** Butcher tableau. **Right:** Equation.

2.1.3 Runge-Kutta 3 scheme

In the same way, we introduce the Runge-Kutta 3 (denoted RK3) method. It calculates two intermediate values (p_2, p_3) to obtain y_{k+1} . See figure 4 for the value of coefficients in the Butcher table and equation (9) for the explicit equations. In this case, the method is of order three in time.

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 1 & -1 & 2 & 0 \\ \hline & 1/6 & 2/3 & 1/6 \end{array} \qquad \begin{array}{l} y_{k+1} = y_k + \frac{\tau}{6} (p_1 + 4p_2 + p_3), \\ p_1 = f(t_k, y_k), \\ p_2 = f(t_{k+1/2}, y_k + \frac{\tau}{2} p_1), \\ p_3 = f(t_{k+1}, y_k + h(-p_1 + 2p_2)). \end{array} \quad (9)$$

Figure 4: Runge-Kutta 3 method. **Left:** Butcher tableau. **Right:** Equation.

2.1.4 Runge-Kutta 4 scheme

The last method is the celebrated Runge-Kutta 4 (denoted RK4) where three intermediate values (p_2, p_3, p_4) are computed to determine y_{k+1} . The value of coefficients is presented in figure 5 and its application to equation (5) is given in equation (10). This method is of order four in time.

0	0	0	0	0	$y_{k+1} = y_k + \frac{\tau}{6} (p_1 + 2p_2 + 2p_3 + p_4),$ $p_1 = f(t_k, y_k),$ $p_2 = f(t_{k+1/2}, y_k + \frac{\tau}{2}p_1),$ $p_3 = f(t_{k+1/2}, y_k + \frac{\tau}{2}p_2),$ $p_4 = f(t_{k+1}, y_k + \tau p_3).$
1/2	1/2	0	0	0	
1/2	0	1/2	0	0	
1	0	0	1	0	
	1/6	1/3	1/3	1/6	

(10)

Figure 5: Runge-Kutta 4 method. **Left:** Butcher tableau. **Right:** Equation.

2.2 Variational approach

Unfortunately, none of the schemes presented in Section 2.1 can be used for finding a MFG equilibrium. Firstly because the problem is not really presented that way, and secondly because the space of the unknowns is, in general, not a vector space but a metric space. Therefore we need first to generalize the Runge-Kutta schemes to metric spaces and then to apply them to the MFG setting.

Let (\mathcal{A}, d) be a metric space. The definition 2.1 below gives the properties of a geodesic space (see [19] for additional details).

Definition 2.1. *A curve $\gamma : [0, 1] \rightarrow \mathcal{A}$ is called a (constant speed) geodesic provided that $d(\gamma(t), \gamma(s)) = |t - s| \cdot d(\gamma(0), \gamma(1))$ and the space is called geodesic if, for any couple of points $(X, Y) \in \mathcal{A}^2$, there exists at least a geodesic γ connecting them, that is, such that $\gamma(0) = X$, $\gamma(1) = Y$.*

From now on we assume that (\mathcal{A}, d) is a geodesic space. Consider $\mathcal{P} : \mathcal{A} \times \mathcal{A} \rightarrow \mathbb{R}$ a function with the following properties:

(H1) $\forall n \leq 4, \forall r > 0, \forall \xi, Y_1, \dots, Y_n \in \mathcal{A}$, the set of vectors

$\{(\mathcal{P}(z, Y_1), \dots, \mathcal{P}(z, Y_n)); z \in \mathcal{A}, d(z, \xi) \leq r\}$ is compact as a subset of \mathbb{R}^n ,

(H2) for any point $Y \in \mathcal{A}$ and any constant speed geodesic γ the function $t \mapsto \mathcal{P}(\gamma(t), Y)$ from $[0, 1]$ to \mathbb{R} is linear.

The evolution equation that we want to solve has the form $\xi'(t) = \mathcal{P}(\cdot, \xi(t))$ (but note that this is only a formal expression as $\xi'(t)$ does not have a well-defined meaning in a general metric space).

This section develops a variational Runge-Kutta method in a metric space. We propose a method that does not assume any vector calculus but uses the

hypothesis **(H2)** which defines the notion of linear application in a metric space (see also [7, Section 8, Definition 8.1 page 480] for more details). As τ tends to zero equation (4) describes a curve. The purpose of the scheme is to describe this evolution faster and more precisely that is to say to obtain high order schemes.

2.2.1 Variational Explicit Euler scheme

The first scheme of that form was introduced in [9, Eq 3.2]. Formally, we define the *variational Explicit Euler scheme (VEE)* by:

$$\xi_{k+1} \in \operatorname{argmin}_{\eta \in \mathcal{A}} \left\{ \frac{d(\eta, \xi_k)^2}{2\tau} + \mathcal{P}(\eta, \xi_k) \right\}. \quad (11)$$

2.2.2 Variational Heun scheme

The *variational Heun scheme (VH)* introduces, as in vector space, an intermediate value $\tilde{\xi}_{k+1}$ (equation (12a)) and uses it to compute ξ_{k+1} (equation (12b)).

$$\tilde{\xi}_{k+1} \in \operatorname{argmin}_{\eta \in \mathcal{A}} \left\{ \frac{d(\eta, \xi_k)^2}{2\tau} + \mathcal{P}(\eta, \xi_k) \right\}, \quad (12a)$$

$$\xi_{k+1} \in \operatorname{argmin}_{\eta \in \mathcal{A}} \left\{ \frac{d(\eta, \xi_k)^2}{2\tau} + \frac{1}{2}\mathcal{P}(\eta, \xi_k) + \frac{1}{2}\mathcal{P}(\eta, \tilde{\xi}_{k+1}) \right\}. \quad (12b)$$

Note that two minimizations are required in order to obtain ξ_{k+1} .

2.2.3 Variational Runge-Kutta 3 scheme

The *variational Runge-Kutta 3 scheme (VRK3)* is defined by equation (13). Two intermediate values are computed in this case ($\tilde{\xi}_{k+1}^1$ with equation (13a) and $\tilde{\xi}_{k+1}^2$ with equation (13b)) in order to obtain ξ_{k+1} using equation (13c).

$$\tilde{\xi}_{k+1}^1 \in \operatorname{argmin}_{\eta \in \mathcal{A}} \left\{ \frac{d(\eta, \xi_k)^2}{2\tau} + \frac{1}{2}\mathcal{P}(\eta, \xi_k) \right\}, \quad (13a)$$

$$\tilde{\xi}_{k+1}^2 \in \operatorname{argmin}_{\eta \in \mathcal{A}} \left\{ \frac{d(\eta, \xi_k)^2}{2\tau} - \mathcal{P}(\eta, \tilde{\xi}_{k+1}^1) + 2\mathcal{P}(\eta, \tilde{\xi}_{k+1}^2) \right\}, \quad (13b)$$

$$\xi_{k+1} \in \operatorname{argmin}_{\eta \in \mathcal{A}} \left\{ \frac{d(\eta, \xi_k)^2}{2\tau} + \frac{1}{6}\mathcal{P}(\eta, \xi_k) + \frac{2}{3}\mathcal{P}(\eta, \tilde{\xi}_{k+1}^1) + \frac{1}{3}\mathcal{P}(\eta, \tilde{\xi}_{k+1}^2) \right\}. \quad (13c)$$

2.2.4 Variational Runge-Kutta 4 scheme

The *variational Runge-Kutta 4 scheme* is presented in equation (14). Three intermediate values ($\tilde{\xi}_{k+1}^1$ with equation (14a), $\tilde{\xi}_{k+1}^2$ with equation (14b) and $\tilde{\xi}_{k+1}^3$ defined by equation (14c)) are computed in order to obtain ξ_{k+1} by using equation (14d).

$$\tilde{\xi}_{k+1}^1 \in \operatorname{argmin}_{\eta \in \mathcal{A}} \left\{ \frac{d(\eta, \xi_k)^2}{2\tau} + \frac{1}{2} \mathcal{P}(\eta, \xi_k) \right\}, \quad (14a)$$

$$\tilde{\xi}_{k+1}^2 \in \operatorname{argmin}_{\eta \in \mathcal{A}} \left\{ \frac{d(\eta, \xi_k)^2}{2\tau} + \frac{1}{2} \mathcal{P}(\eta, \tilde{\xi}_{k+1}^1) \right\}, \quad (14b)$$

$$\tilde{\xi}_{k+1}^3 \in \operatorname{argmin}_{\eta \in \mathcal{A}} \left\{ \frac{d(\eta, \xi_k)^2}{2\tau} + \frac{1}{2} \mathcal{P}(\eta, \tilde{\xi}_{k+1}^2) \right\}, \quad (14c)$$

$$\xi_{k+1} \in \operatorname{argmin}_{\eta \in \mathcal{A}} \left\{ \frac{d(\eta, \xi_k)^2}{2\tau} + \frac{1}{6} \mathcal{P}(\eta, \xi_k) + \frac{1}{3} \mathcal{P}(\eta, \tilde{\xi}_{k+1}^1) + \frac{1}{3} \mathcal{P}(\eta, \tilde{\xi}_{k+1}^2) + \frac{1}{6} \mathcal{P}(\eta, \tilde{\xi}_{k+1}^3) \right\}. \quad (14d)$$

Note that four minimizations are needed in order to obtain ξ_{k+1} .

See section 3.2 for a numerical application and the study of the order in time of these schemes.

2.3 Property of variational scheme

In this subsection we prove that using hypotheses **(H1)** and **(H2)**, the variational schemes introduced above are well-defined (Prop. 2.1) and correspond, when the ambient space is Hilbert, to the Runge-Kutta method presented in section 2.1 (Prop. 2.2).

Prop 2.1. *Under the hypothesis **(H1)** and **(H2)**, the equations (11), (12), (13) and (14) defining respectively the VEE, VH, VRK3 and VRK4 schemes admit a solution, i.e., the schemes are well defined.*

Proof. As the argumentation is very similar for all schemes, we present the general case where $\xi_{k+1} \in \operatorname{argmin}_{\eta \in \mathcal{A}} \{\mathcal{F}(\eta)\}$ with $\mathcal{F} : \mathcal{A} \rightarrow \mathbb{R}$, for fixed $\xi \in \mathcal{A}$, $\mathcal{F}(\eta) = \frac{d(\eta, \xi)^2}{2\tau} + l(\eta)$ where l satisfies hypothesis **(H2)** and the following hypothesis **(H1bis)**:

(H1bis) $\forall r > 0, \forall \xi \in \mathcal{A}$, the set $\{l(z); z \in \mathcal{A}, d(z, \xi) \leq r\}$ is compact as a subset of \mathbb{R} .

We will prove that the application \mathcal{F} attains its minimum in \mathcal{A} .

Let $(z_k)_{k \in \mathbb{N}} \in \mathcal{A}$ be a sequence such that $\lim_{k \rightarrow \infty} \mathcal{F}(z_k) = m$ with $m = \inf_{\eta \in \mathcal{A}} \mathcal{F}(\eta)$. We show that $d(z_k, \xi)$ is bounded then we find a minimizer.

Suppose $d(z_k, \xi) = \lambda > 1$ and let γ be the geodesic connecting ξ and z_k ($\gamma(0) = \xi$ and $\gamma(1) = z_k$). Consider an element in the geodesic $z = \gamma(t)$ such that $d(z, \xi) = 1$ (implies necessary $t = 1/\lambda$) and using hypothesis **(H2)**, we obtain:

$$l(z) = \left(1 - \frac{1}{\lambda}\right)l(\xi) + \frac{1}{\lambda}l(z_k). \quad (15)$$

For k large enough, z_k is such that $\mathcal{F}(z_k) < 2m$ that is $\frac{\lambda^2}{2\tau} + l(z_k) < 2m$. Rearranging equation (15) gives $l(z_k) = \lambda l(z) - (\lambda - 1)l(\xi)$, note that $l(\xi)$ is constant and as $d(z, \xi) = 1$, hypothesis **(H1bis)** insures that $l(z)$ is bounded, so $l(z_k)$ is also bounded (by $M \in \mathbb{R}$). Consequently, there exists a constant C , depending on m, τ and M such that $\lambda < C$.

As $d(z_k, \xi)$ is bounded, there exists a converging subsequence, $(x_k)_{k \in \mathbb{N}} \in \mathcal{A}$ such that $d(x_k, \xi) \rightarrow d_1$, and $l(x_k)$ converges to $m - \frac{d_1^2}{2\tau}$. Starting from some index k , $x_k \in B(\xi, d_1)$ (the ball with center ξ and radius d_1) and if it is not the case, we replace x_k by the element at the intersection of the ball and the geodesic γ linking x_k and ξ . This operation does not change the limit of $l(z_k)$: noting temporarily \tilde{x}_k the obtained sequence, as l satisfies hypothesis **(H2)**, we have $l(\tilde{x}_k) = \left(1 - \frac{d_1}{d(x_k, \xi)}\right)l(\xi) + \frac{d_1}{d(x_k, \xi)}l(x_k)$ with $d(x_k, \xi) \rightarrow d_1$. By hypothesis **(H1bis)**, the set $l(x_k)$ is closed, so there exists an element $Z \in B(\xi, d_1)$ such that $l(Z) = m - \frac{d_1^2}{2\tau}$ with, of course, $d(Z, \xi) \leq d_1$. In this case, $\mathcal{F}(Z) = \frac{d(Z, \xi)^2}{2\tau} + m - \frac{d_1^2}{2\tau} \leq m$, so Z is a minimizer.

Let $n \leq 4$, $Y_1, \dots, Y_n \in \mathcal{A}$, $\lambda_1, \dots, \lambda_n \in \mathbb{R}$ and \mathcal{P} satisfying **(H1)** and **(H2)**. We define the linear combination l of \mathcal{P} by : $l(\eta) = \sum_{i=1}^n \lambda_i \mathcal{P}(\eta, Y_i)$. We show that l satisfies **(H1bis)** and **(H2)**. As all elements of the sum are in a compact set, the sum is bounded. Let $(z_k)_{k \in \mathbb{N}} \in \mathcal{A}$ be a sequence such that $\lim_{k \rightarrow \infty} l(z_k) = \alpha$. Using **(H1)**, there exists a subsequence of z_k (also noted z_k) such that the element $(\mathcal{P}(z_k, Y_1), \dots, \mathcal{P}(z_k, Y_n)) \in \mathbb{R}^n$ converges to $(\alpha_1, \dots, \alpha_n)$ so $l(z_k)$ converges to $l(z)$ with $l(z) = \sum_{i=1}^n \lambda_i \alpha_i = \alpha$.

It is left to the reader to show the equivalence of hypotheses **(H1)** and **(H1bis)** for l . \square

Prop 2.2. *Let \mathcal{H} be a Hilbert space, $f : \mathcal{H} \rightarrow \mathcal{H}$ be a function and $\mathcal{P}(x, y) = \langle x, f(y) \rangle$. Then the schemes VEE (equation (11)), VH (equation (12)), VRK3 (equation (13)), and VRK4 (equation (14)) correspond to Explicit Euler (equation (7)), Heun (equation (8)), Runge-Kutta 3 (equation (9)) and Runge-Kutta 4 (equation (10)) schemes respectively for the evolution equation (5).*

Proof. We prove hypothesis **(H1)** in the case $n = 1$, the proof for the general case is left to the reader. We show that, for $\xi \in \mathcal{H}$, $\mathcal{D} = \{\langle z, f(\xi) \rangle; z \in$

$\mathcal{H}, d(z, \xi) \leq r\}$ is bounded and closed. Denoting $\|\cdot\|$ the norm of \mathcal{H} , by the triangular inequality when $x \in B(\xi, r)$, $\|x\| \leq r + \|\xi\|$. For $x \in \mathcal{D}$, $\|\langle x, f(\xi) \rangle\| \leq \|x\| \cdot \|f(\xi)\| \leq (r + \|\xi\|) \cdot \|f(\xi)\| < \infty$, so \mathcal{D} is bounded. Let z be an element of $B(\xi, r)$ and $x \in \mathcal{H}$ such that $z = \xi + x$ with $\|x\| \leq r$, by linearity $\langle z, f(\xi) \rangle = \langle \xi, f(\xi) \rangle + \langle x, f(\xi) \rangle$. Furthermore, $\langle x, f(\xi) \rangle \leq \|x\| \cdot \|f(\xi)\| \leq r\|f(\xi)\|$ so $\{\langle z, f(\xi) \rangle, z \in B(\xi, r)\}$ is included in the closed interval $[\langle \xi, f(\xi) \rangle - r\|f(\xi)\|, \langle \xi, f(\xi) \rangle + r\|f(\xi)\|]$. If we take $x = \lambda \frac{f(\xi)}{\|f(\xi)\|}$ with $\lambda \in [-r, r]$ then $\langle x, f(\xi) \rangle = \lambda\|f(\xi)\|$ which implies $\langle z, f(\xi) \rangle = \langle \xi, f(\xi) \rangle + \lambda\|f(\xi)\|$. Therefore $\{\langle z, f(\xi) \rangle, z \in B(\xi, r)\}$ is exactly $[\langle \xi, f(\xi) \rangle - r\|f(\xi)\|, \langle \xi, f(\xi) \rangle + r\|f(\xi)\|]$ and is closed as a closed interval of \mathbb{R} .

To prove hypothesis **(H2)**, consider $x_0, x_1 \in \mathcal{H}$ and for $t \in [0, 1]$, $\gamma(t) = tx_1 + (1-t)x_0$ the segment between x_0 and x_1 . For $t, s \in [0, 1]$, with straightforward computation, we have $d(\gamma(t), \gamma(s)) = |t - s| \cdot d(\gamma(0), \gamma(1))$, showing that γ is a (constant speed) geodesic. Assume that there exists another geodesic γ_2 linking x_0 and x_1 . Let $z = \gamma_2(t)$ be an element only on γ_2 ; using the triangle inequality and that γ is the segment linking x_0 and x_1 we have $d(x_0, z) + d(z, x_1) > d(x_0, x_1)$. Furthermore as γ_2 is a geodesic, left member of previous equation is $td(x_0, x_1) + (1-t)d(x_0, x_1) = d(x_0, x_1)$. We obtain a contradiction thus there does not exist another geodesic. The function $t \rightarrow \mathcal{P}(\gamma(t), Y)$ has the form $t \rightarrow \langle tx_1 + (1-t)x_0, f(Y) \rangle$, so is linear.

We now prove the equivalence of schemes. The scheme *VEE* is defined by the following equation:

$$\xi_{k+1} \in \operatorname{argmin}_{\eta \in \mathcal{H}} \left\{ \frac{\|\eta - \xi_k\|^2}{2\tau} + \langle \eta, f(\xi_k) \rangle \right\}.$$

The application $\mathcal{F} : \mathcal{H} \rightarrow \mathbb{R}$, $\mathcal{F}(\eta) = \frac{\|\eta - \xi_k\|^2}{2\tau} + \langle \eta, f(\xi_k) \rangle$ is differentiable and its derivative $\mathcal{F}' : \mathcal{H} \rightarrow \mathcal{H}$ is $\mathcal{F}'(\eta) = \frac{\eta - \xi_k}{\tau} + f(\xi_k)$. The minimizer of \mathcal{F} is a critical point, the minimum noted ξ_{k+1} , satisfies $\mathcal{F}'(\xi_{k+1}) = 0$. After trivial rearrangement, we obtain $\xi_{k+1} = \xi_k - \tau f(\xi_k)$, that is the Explicit Euler scheme presented in (7) for equation (5). Arguments are similar for other schemes. \square

3 Numerical illustration

3.1 Framework

F. Salvarani and G. Turinici [9] introduced an epidemiological model with possibility of vaccine which has imperfect efficiency and limited persistence. To model the spread of the disease in the population, they use a compartmental model and a probability distribution to reflect the individual decisions. The

reader is invited to refer to their article for more details and proofs. A short presentation of the model is also provided in Appendix A.

To find stable individual decision they define the problem as a Nash equilibrium. They find the probability distribution ξ making an individual indifferent to change his vaccination decision if all individuals have the same ξ (see [9, Theorem 2.1] for the proof of equilibrium existence).

Let \mathcal{C}_ξ be the cost of pure strategies "vaccination happens at time t " when all individuals choose as vaccination strategy ξ . In that case $\langle \eta, \mathcal{C}_\xi \rangle$ represents the cost of an individual with strategy η when others use strategy ξ .

The definition of the mapping $E(\xi)$ as introduced in [9] is *the maximum gain obtained by an individual if he changes unilaterally his strategy and everybody else remains with the strategy ξ* ; with mathematical notation:

$$E(\xi) = \langle \xi, \mathcal{C}_\xi \rangle - \min_{\eta \in \Sigma_{N+1}} \langle \eta, \mathcal{C}_\xi \rangle.$$

where $\Sigma_{N+1} = \left\{ x \in \mathbb{R}^{N+1} \mid \sum_{k=0}^N x_k = 1 \text{ and } x_k \geq 0, 0 \leq k \leq N \right\}$. A minimum of the mapping $\xi \rightarrow E(\xi)$ is a Nash equilibrium. To find it they introduce an iterative method depending on a step τ (algorithm 1). In this algorithm, equation (16) is used. The following intuitive interpretation is also provided: an individual in a population with strategy ξ_k will, if necessary, adjust his strategy to minimize his cost function $\eta \rightarrow \langle \eta, \mathcal{C}_{\xi_k} \rangle$ while at the same time keeping small the distance between the previous strategy ξ_k and the new ξ_{k+1} . But algorithm 1 can also be seen as numerical resolution of an evolution e.g., describing a curve in the metric space of the admissible strategies. That is why we apply variational methods in the metric space Σ_{N+1} with the standard Euclidean distance to obtain faster convergence to the Nash equilibrium. Here $\mathcal{P}(x, y) = \langle x, \mathcal{C}_y \rangle$ and for the same reasons as in the proof of Prop. 2.2, \mathcal{P} satisfies hypotheses **(H1)** and **(H2)**. Note that with high order schemes *VH*, *VRK3* and *VRK4*, we lose the intuitive idea but we increase the Nash equilibrium computing.

Algorithm 1 Finding a Nash equilibrium (as introduced in [9])

- 1: Choose a step $\tau > 0$ and a starting distribution ξ_0 .
- 2: Set iteration count $k = 1$.
- 3: Compute ξ_{k+1} with following formula:

$$\xi_{k+1} \in \operatorname{argmin}_{\eta \in \Sigma_{N+1}} \left\{ \frac{d(\eta, \xi_k)^2}{2\tau} + \langle \eta, \mathcal{C}_{\xi_k} \rangle \right\}. \quad (16)$$

- 4: If $E(\xi_{k+1})$ is smaller than a given *tolerance* then stop and exit, otherwise set $k \rightarrow k + 1$ and go back to step 3.
-

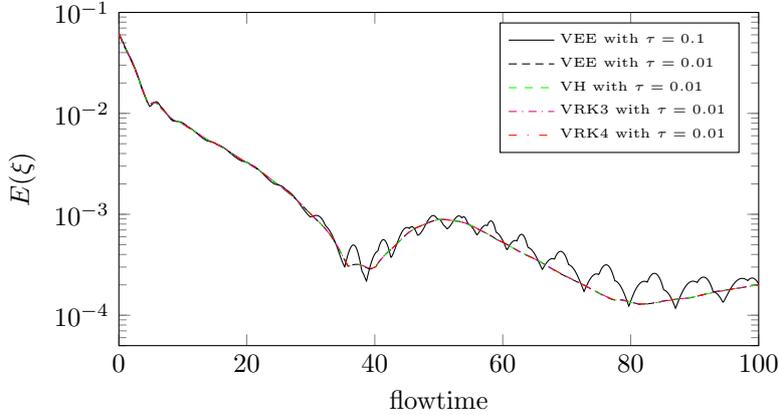


Figure 6: The evolution of the mapping $E(\cdot)$ for the four schemes in section 2.2 in the case *Short persistence, large efficacy*. In [9] VEE with $\tau = 0.1$ is used.

3.2 Results

In this section we test the variational schemes proposed in section 2.2.

The reader is invited to refer to [9, Sec 4.6] or Appendix A for the numerical values of the two studied cases *Short persistence, large efficacy* (with vaccine persistence at one month with a delay of action at five days) and *Long persistence, 100% efficacy* (with persistence of the vaccine at six months with no delay of action).

In order to appreciate the convergence scheme for the case *Short persistence, large efficacy* the evolution of the mapping $E(\cdot)$ is presented (see figure 6 for VEE with $\tau = 0.1$), where the evolution for the four schemes with lower τ value is added to stabilize result of mapping $E(\cdot)$.

For the *Short persistence, large efficacy* case, the graph at the left in figure 7 presents the numerical estimation of the scheme order: only the VEE is of order one, the others are of order two in τ . Recall that a high order scheme needs a very regular functional to provide high order convergence, but in our case the regularity of the function is completely unknown. However, this case remains very interesting because it shows that even if the regularity of the function is not enough to obtain order three or four, the $VRK3$ and $VRK4$ still improve the regularity of the function and have a better order than the VEE scheme.

For the other example *Long persistence, 100% efficacy*, the convergence is faster: figure 8 compares the evolution of mapping $E(\cdot)$ for the two cases. In the second case, the graph at the right of figure 7 shows that the scheme has high order as it was expected previously. VH is indeed of order 2 and $VRK3$ and $VRK4$ are respectively order three and four.

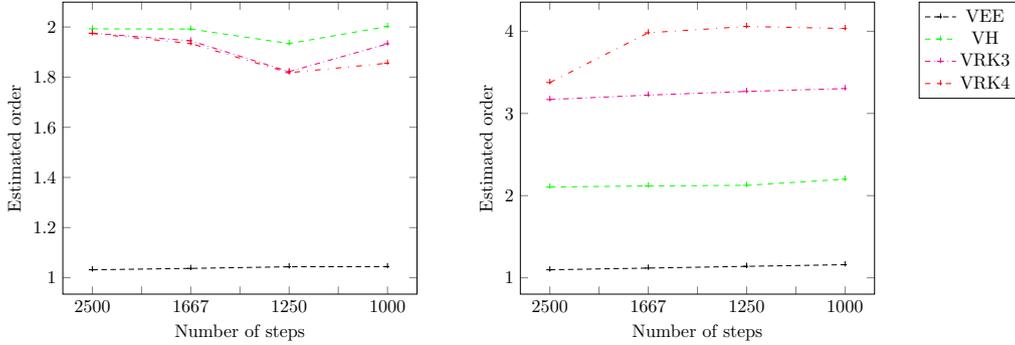


Figure 7: Numerical order obtained for the four presented schemes. Reference solution is given by a $VRK4$ scheme with $\tau_{ref} = 0.01$. Other steps used are 0.04, 0.06, 0.08, 0.10 and 0.12. **Left:** *Short persistence, large efficacy*. **Right:** *Long persistence, 100% efficacy*.

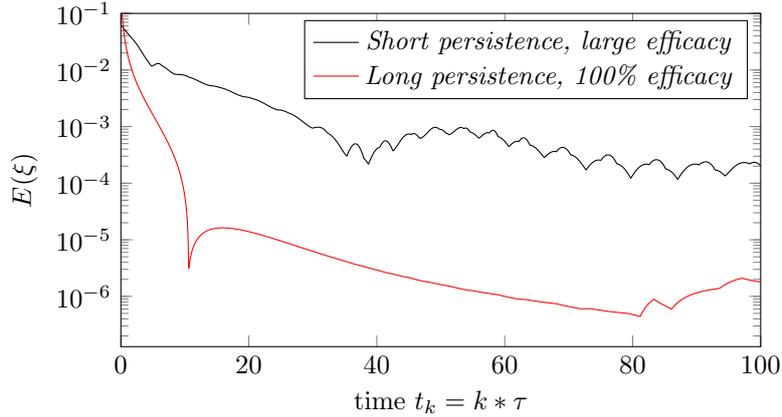


Figure 8: Mapping $E(\cdot)$ for the case *Short persistence, large efficacy* and *Long persistence, 100% efficacy*, generated with VEE scheme and $\tau = 0.1$.

4 Perspectives

This work introduces three high order schemes to find a Nash equilibrium and illustrates their use in an epidemiological application.

We show numerically that the schemes VH , $VRK3$ and $VRK4$ exhibit better order than VEE and we can obtain, depending on the regularity of the function, up to order four convergence. The approach based on the Runge-Kutta method can be applied for other numerical schemes, for instance Mid Point, Leap-Frog or Adams-Bashford methods. Please note that presented algorithms are not optimized, as minimizations can take a long time and need a high numerical precision, so the time execution can be significant. A perspec-

tive of this work is to provide an extension to bi-dimensional or tri-dimensional problems.

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A Presentation of the epidemiological model

This section reproduces a short presentation of the epidemiological model and of the cost computing as introduced in [9, Sec 2]. Please refer to the original article for more details and proof.

A.1 Epidemiological model

The model simulates the dynamics of an epidemic in a population. The final time period T is supposed finite, and the time horizon can be discretized in $(N + 1)$ time instants, noted $t_0 = 0, t_1 = \Delta T, \dots, t_N = T$.

The model is compartmental, and the population is divided into several classes: *susceptible individuals* (S_n) is the proportion of individuals susceptible to catch the disease at time instant t_n ; *infected individuals* regroups individuals who are infected, more precisely, I_n^ω is the proportion of individuals who have been infected at time instant $t_{n-\omega}$ (with $\omega \in \{0, 1, \dots, \Omega\}$) and I_n is the sum of all I_n^ω ; *recovered individuals* (R_n) is the proportion of individuals who have exited from one infected class; *vaccinated individuals* (V_n^θ where θ counts the time between vaccination time instant and current time instant with $\theta \in \{0, 1, \dots, \Theta\}$) is the proportion of vaccinated individuals at time instant t_n and not infected since; *failed vaccinated individuals* (F_n) is the proportion of individuals who were vaccinated at some time $t \leq t_n$ but whose vaccination failed and have not been infected since. As individuals can only take vaccination once, V_n^Ω represents individuals who have lost immunity. Lastly U_n represents the proportion of individuals vaccinated between t_n and t_{n+1} , a proportion f of them will never develop any immunity and go to the *failed vaccination* class.

The specificities of disease are represented by the vector $\gamma = (\gamma^0, \dots, \gamma^\Omega) \in (\mathbb{R}_+)^{\Omega+1}$ (which reflects the recovery of an infected individual); the function

$\beta(t)$ (which characterizes the contact between an infected individual and a susceptible one at time t); and the vector $\alpha \in [0, 1]$ which quantifies the protection provided by the vaccine in terms of the probability of infection.

The model is defined by the following system of equations:

$$S_{n+1} = (1 - \beta_{\Delta T}^n I_n) (S_n - U_n) \quad (17a)$$

$$I_{n+1}^0 = \beta_{\Delta T}^n \left[F_n + S_n + \sum_{\theta=0}^{N-1} \alpha_\theta V_n^\theta \right] I_n \quad (17b)$$

$$I_{n+1}^{\omega+1} = (1 - \gamma_{\Delta T}^\omega) I_n^\omega \quad \omega = 0, \dots, \Omega - 1 \quad (17c)$$

$$V_{n+1}^0 = (1 - f) \cdot (1 - \beta_{\Delta T}^n I_n) U_n \quad (17d)$$

$$V_{n+1}^{\theta+1} = (1 - \beta_{\Delta T}^n \alpha_\theta I_n) V_n^\theta, \quad \theta = 0, \dots, \Theta - 2 \quad (17e)$$

$$V_{n+1}^\Theta = (1 - \beta_{\Delta T}^n \alpha_{\Theta-1} I_n) V_n^{\Theta-1} + (1 - \beta_{\Delta T}^n I_n) V_n^\Theta \quad (17f)$$

$$F_{n+1} = f \cdot (1 - \beta_{\Delta T}^n I_n) U_n + F_n (1 - \beta_{\Delta T}^n I_n) \quad (17g)$$

with initial conditions:

$$S_0 = S_{0-}, \quad I_0^\omega = I_{0-}^\omega, \quad V_0^\theta = 0, \quad \forall \theta \geq 0. \quad (17h)$$

A.2 Individual cost

The system (17) presents the spread of the disease at the population level. For an individual, we consider the Markov chain M_n which describes, in terms of transition probabilities (see [9, Eq 2.10]), the state of the individual ($M_n \in \{S, R, F, I^j, V^l\}$ with $j \in \{0, \dots, \Omega\}$ and $l \in \{0, \dots, \Omega\}$).

In order to reflect the decision of an individual, we introduce the probability density ξ defined on $\{t_0, \dots, t_{N-1}\} \cup \infty$. In practice, before the epidemic starts, the individual chooses his probability of vaccination at each time step t_k , assuming his non-infected status.

The collection of conditional rates $\lambda = (\lambda_n)_{n=1}^N$ is given by the density ξ :

$$\forall n \leq N - 1 : \lambda_n = \begin{cases} \frac{\xi_n}{\xi_n + \dots + \xi_\infty}, & \text{if } \xi_n + \dots + \xi_\infty > 0 \\ 0, & \text{otherwise} \end{cases} \quad (18)$$

The individual in the susceptible class at time t_0 ($M_0 = S$) has the following cost: $J_{indi}(\xi; U) = \langle \xi, \mathcal{C}_U \rangle$ where \mathcal{C}_U (the vector representing the cost of all

pure strategies "vaccination sure at time t ") is defined by:

$$\mathcal{E}_U(t_n) = \begin{cases} r_I \varphi_n^I + (1 - \varphi_n^I)(r_V + (1 - f)r_I \varphi_n^{V,I}) + r_I f(\varphi_\infty^I - \varphi_n^I) & \text{for } n < N, \\ r_I \varphi_\infty^I & \text{for } n = N. \end{cases} \quad (19)$$

Here $\varphi_n^{V,I} = 1 - \prod_{k=n}^{\ominus} (1 - \beta_{\Delta T}^k \alpha_{k-n-1} I_k)$, with the convention $\alpha_{-1} = 1$ and $\varphi_n^I = 1 - \prod_{k=0}^n (1 - \beta_{\Delta T}^k I_k)$ (for $n = 0, \dots, N-1$), $\varphi_\infty^I = 1 - \prod_{k=0}^N (1 - \beta_{\Delta T}^k I_k)$.

The equilibrium between individual dynamics and global dynamics (17) is attained when $U_n = \lambda_n S_n$.

The purpose of an individual is to minimize $J_{indi}(\xi; U)$ under the constraint $\xi_0 + \xi_1 + \dots + \xi_{N-1} + \xi_\infty = 1$ and $\xi_k \geq 0$.

A.3 Numerical values

This section describes the numerical values used in the two cases presented in this paper: *Short persistence, large efficacy* and *Long persistence, 100% efficacy*. These values are sensibly similar to the ones used in [9, Subsec 4.2 and 4.3].

For the epidemic parameters, we consider a total simulation time at one year ($T = 1$); three time instants by day ($N = 365 * 3$); a recovery rate $\gamma^\omega = 365/3.2$ ($\Omega = 20$); the reproduction number $R_0 = 1.35$ thus $\beta = \gamma R_0$; $t_2^\beta = 1/2$ such that $\beta(t) = \beta$ for $t \leq t_2^\beta$ and then $\beta(t) = \beta_{min}$ for $t > t_2^\beta$ where $\beta_{min} = \gamma/S_0$; the relative cost of the epidemic is $r_I = 1$.

Finally, we introduce t_1^α , t_2^α and set $\alpha_\theta = 1 - \mathbf{1}_{[t_1^\alpha, t_2^\alpha]}$. For the case *Short persistence, large efficacy*, $t_1^\alpha = 5/365$ and $t_2^\alpha = 1/12$ ($\Omega = 93$). For the case *Long persistence, 100% efficacy*, $t_1^\alpha = 0$ and $t_2^\alpha = 1/2$ ($\Omega = 549$). We suppose a failure rate $f = 0$, and the relative cost of the vaccination $r_V = 0.005$.

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L.L: Université Paris-Dauphine, PSL Research University, CNRS, UMR [7534], CEREMADE, 75016 PARIS, FRANCE & BIOEPAR, INRA-Oniris, 44307 Nantes, France.

E-mail adress : `laetitia.laguzet@oniris-nantes.fr`