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GEOMETRIC INTEGRATION METHODS THAT PRESERVE LYAPUNOV FUNCTIONS *

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Abstract.

We consider ordinary differential equations (ODEs) with a known Lyapunov function V. To ensure that a numerical integrator reflects the correct dynamical behaviour of the system, the numerical integrator should have V as a discrete Lyapunov function. Only second-order geometric integrators of this type are known for arbitrary Lyapunov functions. In this paper we describe projection-based methods of arbitrary order that preserve any given Lyapunov function.

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Key words: Geometric integration, Lyapunov function, Runge-Kutta methods, numerical solution.

1 Introduction

In recent years there has been tremendous interest in *geometric integration*, i.e. the numerical integration of differential equations while preserving some (geometric) property of the system exactly (that is, to machine precision). Some examples of geometric properties that can be preserved exactly are: first integrals, symmetries and reversing symmetries, phase-space volume, symplectic structure, contact structure, foliations, Lie group structure, etc. Surveys of geometric integration are given in Budd & Iserles [2], Budd & Piggott [3], Hairer, Lubich & Wanner [9], Iserles, Munthe-Kaas, Nørsett & Zanna [11], Leimkuhler & Reich [13], McLachlan & Quispel [17], [18] and Sanz-Serna & Calvo [19].

In this paper we consider integrators that exactly preserve a given Lyapunov function. The system of ordinary differential equations

$$\dot{y} = f(y), \qquad y(t_0) = y_0 \tag{1.1}$$

is said to have the *Lyapunov function* V in a region $B \subset I\!R^N$, if $\dot{V} \leq 0$, i.e. if

$$\alpha(y) := \nabla V(y) \cdot f(y) \leq 0,$$

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holds in this region and V is bounded from below. The Lyapunov function is called *strict* if $<$ holds outside the set of equilibrium points

$$E := \{y \mid f(y) = 0\}.$$

The numerical method

$$y_{n+1} = \Phi_h(y_n), \tag{1.2}$$

is said to have the *Lyapunov function* V, if

$$V(y_{n+1}) \leq V(y_n).$$

The Lyapunov function is called *strict* if $<$ holds outside the set of fixed points

$$E_h := \{y \mid \Phi_h(y) = y\}.$$

A geometric integrator for a system of ordinary differential equations with a Lyapunov function V should preserve V as a Lyapunov function for the discrete system. The Lyapunov function V describes regions of stability, given by the contour lines of V, that can be entered but not left by solutions of the ODE (see e.g. [21]). To ensure that the numerical method has the same regions of stability, V should be a discrete Lyapunov function for the numerical method.

As far as we are aware, the order of accuracy of currently known methods that have this property for general Lyapunov functions (cf. [15],[16]) or for special cases like gradient systems (cf. [4], [21]) is at most two. In fact, in Section 6 of [18] the development of effective methods of order higher than 2 for systems that evolve in a semigroup (of which systems with Lyapunov functions are one case) is given as open problem number 10. This is because composition methods of higher order than two necessarily involve negative time-steps and hence cannot be used for semigroups.

In this paper, we present new projection-based methods of arbitrarily high order, that can preserve an arbitrary (smooth) Lyapunov function. This approach is quite flexible and can easily be extended to ODEs with more than one Lyapunov function. Multiple Lyapunov functions arise frequently in control theory (cf. [12], [14]). Our main results, presented in Section 2, concern Runge-Kutta methods, which form a large and well understood class of methods that can be used efficiently with projection. These methods preserve the nonlinear regions of stability given by the Lyapunov function. It is sometimes favourable to preserve additional structures. A symmetrised projection is presented in Section 3 and it is shown that the symmetric projection methods can preserve linear reversing symmetries in contrast to the non-symmetric projection methods in Section 2. The numerical experiments in Section 4 indicate a very good behaviour of the Lyapunov-preserving methods. It is remarkable that the preservation of the Lyapunov function not only guarantees the expected nonlinear stability, but also improves the trajectories far from equilibrium points. Finally, we give a conclusion in Section 5.

2 Projection methods

Our main idea for obtaining a Lyapunov-preserving method of higher order is to approximate $V(y(t_{n+1}))$ by $V_{n+1} \leq V(y(t_n))$ and to project the computed value $\tilde{y}_{n+1}$ onto the manifold $V(y) = V_{n+1}$.

We describe the approach in more detail by using what we call "the projected Euler method" as a simple example. Besides the usual approximation

$$\tilde{y}_{n+1} = y_n + hf(y_n)$$

we compute an approximation to $V(y(t_{n+1}))$ here by using

$$V_{n+1} = V(y_n) + h\alpha(y_n).$$

Since $\alpha(y) \leq 0$ for all y, it follows that $V_{n+1} \leq V(y_n)$. After that, we project $\tilde{y}_{n+1}$ orthogonally onto the manifold $V(y) = V_{n+1}$, hence the projected value y_{n+1} satisfies $V(y_{n+1}) = V_{n+1} = V(y_n) + h\alpha(y_n) \leq V(y_n)$. This means V is also a Lyapunov function for our method. The approximations $\tilde{y}_{n+1}$ and V_{n+1} are of first order as well as the overall method.

This procedure can be done for fairly general types of methods but we will describe only "projected Runge-Kutta methods". Without loss of generality, here we describe only the first step (i.e. from y_0 to y_1). The approach for an arbitrary Runge-Kutta method of order p given by the tableau

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$

with **non-negative** weights b_i (i.e. $b_i \geq 0$), $i = 1, \ldots, s$, where s is the number of stages, is as follows:

Step 1 Compute the Runge-Kutta approximation

$$g_i = y_0 + h \sum_{j=1}^{s} a_{ij} f(g_j), \qquad i = 1 \ldots s,$$

$$\tilde{y}_1 = y_0 + h \sum_{i=1}^{s} b_i f(g_i).$$

Step 2 Compute the approximation for the Lyapunov function

$$V_1 = V(y_0) + h \sum_{i=1}^{s} b_i \alpha(g_i).$$

Step 3 To get y_1, project $\tilde{y}_1$ orthogonally onto the manifold

$$r(y) := V(y) - V_1 = 0.$$

If $\nabla V(y_0) = 0$, the projection steps 2 and 3 are omitted. In addition, set $y_1 = y_0$ and stop the numerical calculation in the case of a strict Lyapunov function. If $\nabla V(y_0) \neq 0$, the projection is computed as suggested in [9], page 107. This idea is simple enough in order to be combined with any step size selection strategy for Runge-Kutta methods. The property of the projected methods to stay in the stability regions and eventually approach equilibrium points is not destroyed by step size selection (in contrast to some other geometric properties). Furthermore, it is easy to include a check for the solvability of the system (4.5) in [9], page 107, which has to be solved for the projection, and to reduce the step size further, if necessary. In the case of a non-strict Lyapunov function, the situation $\nabla V(y_0) = 0$, but $f(y_0) \neq 0$ might occur. In this case, steps 2 and 3 are omitted and we suggest to solve the minimization problem

$$\|y_1 - \tilde{y}_1\| \to \min \quad \text{subject to} \quad V(y_1) \leq V(y_0).$$

This problem always has a solution that is $\mathcal{O}(h^{p+1})$-close to the exact solution, where p is the order of the underlying Runge-Kutta method. This way neither the order of the method nor the property, that V is a discrete Lyapunov function for the numerical method, is affected. But to simplify the proofs, we will only discuss strict Lyapunov functions in the remainder of this paper. The basic properties of the projected methods are described in the following Theorems 2.1 and 2.2.

THEOREM 2.1. *For a projected Runge-Kutta method the local error satisfies*

$$\|V_1 - V(y(t_0 + h))\| = \mathcal{O}(h^{p+1}), \quad \|y_1 - y(t_0 + h)\| = \mathcal{O}(h^{p+1}), \tag{2.1}$$

where p is the order of the underlying Runge-Kutta method. If V is a strict Lyapunov function and the weights b_i of the Runge-Kutta method are non-negative (positive) then V is a discrete (strict) Lyapunov function for the numerical method.

PROOF. Applying the Runge-Kutta method of order p to the augmented system

$$\begin{array}{rcl} \dot{y} & = & f(y) \\ \dot{V} & = & \alpha(y) \end{array} \tag{2.2}$$

shows, that

$$\|V(y(t_0 + h)) - V_1\| = \mathcal{O}(h^{p+1}). \tag{2.3}$$

If $\nabla V(y_0) = 0$ and there is no projection, the second statement in (2.1) is obvious. If we project, then the distance of $\tilde{y}_1$ to the manifold $V(y) = V(y(t_0 + h))$ is the size of the local error. This observation and (2.3) imply that the convergence does not deteriorate under projection. Hence

$$\|y_1 - y(t_0 + h)\| = \mathcal{O}(h^{p+1}).$$

If all weights b_i are non-negative, we have

$$V(y_1) - V(y_0) = V_1 - V(y_0) = h \sum_{i=1}^{s} b_i \underbrace{\alpha(g_i)}_{\leq 0} \leq 0.$$

Hence V is a discrete Lyapunov function. If the weights are positive and we have $V(y_1) = V(y_0)$, it follows that $\alpha(g_i) = 0$ for all i and hence that $f(g_i) = 0$, since V is strict. This implies $\tilde{y}_1 = y_0$. Now there are two cases. Either $\nabla V(y_0) = 0$ and there is no projection step or $\nabla V(y_0) \neq 0$. In the second case, the projection step has the unique solution $\lambda = 0$ and $y_1 = \tilde{y}_1 = y_0$. In both cases $y_1 = y_0$ and hence V is a strict Lyapunov function for the numerical method. □

There are Runge-Kutta methods of arbitrary order with positive weights. The s-stage Gauss methods are of order $2s$ and the weights are positive. A more detailed study about Runge-Kutta methods based on quadrature formulas with positive weights can be found in [7], chap. IV.13.

Theorem 2.2. *If V is a strict Lyapunov function for the ODE* (1.1) *and the weights of the projected Runge-Kutta method are positive then $E = E_h$, i.e. the equilibrium points of the system coincide with the fixed points of the numerical method.*

Proof. Let $y_0 \in E$. We have to consider the two cases $\nabla V(y_0) = 0$ and $\nabla V(y_0) \neq 0$. In the first case, projection is avoided and y_1 is set to y_0, hence $y_1 = y_0 = \Phi_h(y_0)$ and $y_0 \in E_h$. If $\nabla V(y_0) \neq 0$, $g_i = y_0$ is a solution of the Runge-Kutta system, $\tilde{y}_1 = y_0$ and $V_1 = V(y_0)$. Hence $\lambda = 0$, $y_1 = y_0$ is a solution after the projection, or $y_1 = \Phi_h(y_0) = y_0$. Hence $y_0 \in E_h$. Now assume $y_0 \in E_h$. Then $V(y_0) = V(\Phi_h(y_0)) = V(y_0) + h\sum_{i=1}^{s} b_i\alpha(g_i)$. Hence $\sum_{i=1}^{s} b_i\alpha(g_i) = 0$ and since $b_i > 0$ and $\alpha(g_i) \leq 0$ we have $\alpha(g_i) = 0$. Since V is a strict Lyapunov function for the system this can only hold if $f(g_i) = 0$. But then $g_i = y_0$ and $f(y_0) = f(g_i) = 0$. Hence $y_0 \in E$. □

Remark: If $f(y) = -\nabla V(y)$, $V(y) \geq 0$ and $V(y) \to \infty$ for $\|y\| \to \infty$, the system (1.1) is called a gradient system. Gradient systems form an important class of systems with a strict Lyapunov function V.

The projected methods are of arbitrarily high order and preserve the global stability given by the Lyapunov function. It is well known that Runge-Kutta methods can have spurious fixed points and that $E = E_h$ does not hold in general (cf. [6]). Theorem 2.2 shows that this cannot happen for the projected Runge-Kutta methods. Every fixed point of Φ_h is an equilibrium point of (1.1), even if the Runge-Kutta method without projection has a spurious fixed point.

3 Symmetric projection methods

The exact flow, ϕ_t, of the differential equation (1.1) satisfies $\phi_t \circ \phi_{-t}(y_0) = y_0$ for all values y_0. The preservation of this structural property is in some cases beneficial for the qualitative correctness of the numerical solution. Numerical methods Φ_h that preserve this property, that is $\Phi_h \circ \Phi_{-h}(y_0) = y_0$, are called symmetric or self-adjoint. There is a strong connection between the symmetry of a method and the preservation of reversing symmetries. A reversing symmetry of the phase flow ϕ_t of (1.1) is an invertible map R that satisfies

$$d\,R(f(y)) = -f(R(y)),$$

where dR denotes the derivative (linearization) of R. Hence the exact flow satisfies

$$R \circ \phi_t = \phi_t^{-1} \circ R. \tag{3.1}$$

We show that the symmetric projected Runge-Kutta methods can preserve linear reversing symmetries, that is

$$R \circ \Phi_h = \Phi_h^{-1} \circ R, \tag{3.2}$$

in the special case where R is an invertible linear transformation $R(y) = Ry$ and $V(Ry) = rV(y)$ ($r \neq 0$) holds, where V is a strict Lyapunov function. Without loss of generality, r can be set to ± 1.

It is possible to obtain symmetric projection methods by combining an approach used by Ascher and Reich to enforce conservation of energy (cf. [1]) and in more general contexts by Hairer (cf. [8]), with the observation that a symmetric method would give a symmetric discretisation of the scalar equation $\dot{V} = \alpha(y(t))$.

The projection method based on a symmetric s-stage Runge-Kutta method reads:

$$\begin{array}{rcl} \tilde{y}_0 &=& y_0 + \nabla V(y_0)^T \lambda \\ g_i &=& \tilde{y}_0 + h \sum_{j=1}^{s} a_{ij} f(g_j) \\ \tilde{y}_1 &=& \tilde{y}_0 + h \sum_{i=1}^{s} b_i f(g_i) \\ y_1 &=& \tilde{y}_1 + \nabla V(y_1)^T \lambda \\ V(y_1) &=& V(y_0) + h \sum_{i=1}^{s} b_i \alpha(g_i). \end{array} \tag{3.3}$$

If $\nabla V(y_0) = 0$, λ is set to 0. If V is a strict Lyapunov function, set $y_1 = y_0$, additionally. The overall method is symmetric and shares the properties stated in Section 2 for the nonsymmetric projection methods. This is summarized in Proposition 3.1.

PROPOSITION 3.1. *For a symmetric projected Runge-Kutta method (3.3) the local error satisfies (2.1), where p is the order of the underlying Runge-Kutta method. The overall method is symmetric. If V is a strict Lyapunov-function and the weights b_i of the Runge-Kutta method are positive, then V is a discrete strict Lyapunov function for the numerical method. Furthermore $E = E_h$.*

PROOF. The existence of a numerical solution is shown first. Let $z := (h, y_1, \lambda, g_1, \cdots, g_s)$. Then the system to be solved for λ, the approximation y_1 and the intermediate stages g_i reads $F(z) = 0$ with

$$F(z) = \begin{cases} g_i - y_0 - \nabla V(y_0)^T \lambda - h \sum_{j=1}^{s} a_{ij} f(g_j), \quad i = 1, \cdots, s \\ y_1 - y_0 - \nabla V(y_0)^T \lambda - \nabla V(y_1)^T \lambda - h \sum_{i=1}^{s} b_i f(g_i) \\ V(y_1) - V(y_0) - h \sum_{i=1}^{s} b_i \alpha(g_i) \end{cases}$$

This system has to be solved for $y_1, \lambda, g_1, \cdots, g_s$ in dependence of h if $\nabla V(y_0) \neq 0$. To show that a solution exists, we show that the assumptions of the implicit function theorem are satisfied. For $z_0 := (0, y_0, 0, y_0, \cdots, y_0)$ it is true that $F(z_0) = 0$ and

$$\frac{\partial F}{\partial(y_1, \lambda, g_1^T, \cdots, g_s^T)}(z_0) = \begin{bmatrix} & -\nabla V(y_0)^T & I & & \\ & \vdots & & \ddots & \\ & -\nabla V(y_0)^T & & & I \\ I & -2\nabla V(y_0)^T & & & \\ \nabla V(y_0) & & & & \end{bmatrix},$$

where I is the $N \times N$ identity matrix and N is the dimension of the system of ordinary differential equations. This matrix of size $(N(s+1)+1) \times (N(s+1)+1)$ is regular if $\nabla V(y_0) \neq 0$. Therefore the implicit function theorem guarantees a solution around $(0, y_0, 0, y_0, \cdots, y_0)$ with respect to h.

Now we study the local error. We omit the trivial case $\nabla V(y_0) = 0$. If the underlying Runge-Kutta method is of order p, the system (2.2) is solved up to $O(h^{p+1})$ exactly. Hence we have $F(h, y(t_0 + h), 0, \tilde{g}_1(h), \cdots, \tilde{g}_s(h)) = O(h^{p+1})$, where the $\tilde{g}_i$ are the intermediate steps for the method without projection. Compared to

$$F(h, y_1(h), \lambda(h), g_1(h), \cdots, g_s(h)) = 0,$$

the implicit function theorem implies $\lambda = O(h^{p+1})$, and (2.1).

The symmetry of the algorithm can be seen as follows. Exchanging $h \leftrightarrow -h$ and $y_0 \leftrightarrow y_1$ in (3.3) gives

$$\begin{aligned} \hat{\tilde{y}}_0 &= y_1 + \nabla V(y_1)^T \hat{\lambda} \\ \hat{g}_i &= \hat{\tilde{y}}_0 - h \textstyle\sum_{j=1}^s a_{ij} f(\hat{g}_j) \\ \hat{\tilde{y}}_1 &= \hat{\tilde{y}}_0 - h \textstyle\sum_{i=1}^s b_i f(\hat{g}_i) \\ y_0 &= \hat{\tilde{y}}_1 + \nabla V(y_0)^T \hat{\lambda} \\ V(y_0) &= V(y_1) - h \textstyle\sum_{i=1}^s b_i \alpha(\hat{g}_i). \end{aligned}$$

The variables $\hat{\lambda}$, $\hat{\tilde{y}}_0$, $\hat{\tilde{y}}_1$, $\hat{g}_i$ can be arbitrarily renamed. If they are replaced by $\hat{\lambda} = -\lambda$, $\hat{\tilde{y}}_0 = \tilde{y}_1$, $\hat{\tilde{y}}_1 = \tilde{y}_0$ and $\hat{g}_i = g_{s+1-i}$, where s is the number of stages in the Runge-Kutta method, we find the formulas

$$\begin{aligned} \tilde{y}_0 &= y_0 + \nabla V(y_0)^T \lambda \\ g_i &= \tilde{y}_0 + h \textstyle\sum_{j=1}^s (b_{s+1-j} - a_{s+1-i,s+1-j}) f(g_j) \\ \tilde{y}_1 &= \tilde{y}_0 + h \textstyle\sum_{i=1}^s b_{s+1-i} f(g_i) \\ y_1 &= \tilde{y}_1 + \nabla V(y_1)^T \lambda \\ V(y_1) &= V(y_0) + h \textstyle\sum_{i=1}^s b_{s+1-i} \alpha(g_i). \end{aligned}$$

Since the underlying Runge-Kutta method is symmetric and therefore its coefficients satisfy (cf. [20], [22]):

$$a_{i,j} = b_{s+1-j} - a_{s+1-i,\, s+1-j}, \qquad b_{s+1-i} = b_i,$$

we end up with the formulas of the original system (3.3). This proves the symmetry of the projected method. The statement that V is a discrete Lyapunov function for the numerical method is proved along the same lines as in Theorem 2.1, and the statement $E = E_h$ along the same lines as in the proof of Theorem 2.2. □

The symmetric projection methods can preserve some linear reversing symmetries in contrast to the projection methods in Section 2. In many interesting situations, where the preservation of these symmetries is important, symmetric methods have to be used. Without loss of generality, r can be set to ± 1 in the following proposition.

PROPOSITION 3.2. *If system (1.1) has the linear reversing symmetry $R(y) = Ry$, with an invertible matrix R, that satisfies $RR^T = I$, and $V(R(y)) = rV(y)$, with $r \neq 0$, where V is a strict Lyapunov function, then the symmetric projected Runge-Kutta methods preserve the reversing symmetry, that is (3.2) holds.*

PROOF. Due to the symmetry of the methods proved in Proposition 3.1, we have $\Phi_{-h} = \Phi_h^{-1}$ and hence (3.2) is proved if

$$R \circ \Phi_h = \Phi_{-h} \circ R$$

can be shown. The statements

$$\frac{1}{r}\nabla V(R(y))^T = R\nabla V(y)^T, \quad r\alpha(y) = -\alpha(R(y)), \tag{3.4}$$

follow by differentiation. After writing down the algorithm (3.3) to compute $y_1 = \Phi_h(y_0)$, multiplying the last line of (3.3) with r, and all other lines with R and using (3.4) and the R-reversibility of the exact flow, we find

$$\begin{aligned}
R\tilde{y}_0 &= Ry_0 + \nabla V(Ry_0)^T \tfrac{\lambda}{r} \\
Rg_i &= R\tilde{y}_0 - h\textstyle\sum_{j=1}^s a_{ij} f(Rg_j) \\
R\tilde{y}_1 &= R\tilde{y}_0 - h\textstyle\sum_{i=1}^s b_i f(Rg_i) \\
Ry_1 &= R\tilde{y}_1 + \nabla V(Ry_1)^T \tfrac{\lambda}{r} \\
V(Ry_1) &= V(Ry_0) - h\textstyle\sum_{i=1}^s b_i \alpha(Rg_i).
\end{aligned}$$

At this point, we see that also the Lyapunov function V preserves the reversing symmetry R. Setting $\hat{\lambda} = r^{-1}\lambda$, $\hat{\tilde{y}}_0 = R\tilde{y}_0$, $\hat{\tilde{y}}_1 = R\tilde{y}_1$, $\hat{g}_i = Rg_i$ and $\hat{y}_1 = Ry_1$, the system reads

$$\begin{aligned}
\hat{\tilde{y}}_0 &= Ry_0 + \nabla V(Ry_0)^T \hat{\lambda} \\
\hat{g}_i &= \hat{\tilde{y}}_0 - h\textstyle\sum_{j=1}^s a_{ij} f(\hat{g}_j) \\
\hat{\tilde{y}}_1 &= \hat{\tilde{y}}_0 - h\textstyle\sum_{i=1}^s b_i f(\hat{g}_i) \\
\hat{y}_1 &= \hat{\tilde{y}}_1 + \nabla V(\hat{y}_1)^T \hat{\lambda} \\
V(\hat{y}_1) &= V(Ry_0) - h\textstyle\sum_{i=1}^s b_i \alpha(\hat{g}_i).
\end{aligned}$$

By comparing this with (3.3), we see

$$\Phi_{-h} \circ R(y_0) = \hat{y}_1 = Ry_1 = R \circ \Phi_h(y_0).$$

□

Adaptive step size selection has to be done more carefully for the symmetric projection methods. Fortunately, it is known how to preserve symmetry and reversibility including step size selection ([9], chap. VIII.2). The symmetric projection methods preserve the nonlinear stability regions given by the Lyapunov function and, in addition, preserve linear reversing symmetries, which satisfy the assumptions in Proposition 3.2.

4 Numerical experiments

In the first experiment, we use the Duffing equation without forcing as a test problem (cf. [5]):

$$\begin{aligned} \dot{x} &= y \\ \dot{y} &= x - x^3 - ay \end{aligned}$$

($a \geq 0$) with the Lyapunov function

$$V(x, y) = \frac{1}{2}y^2 - \frac{1}{2}x^2 + \frac{1}{4}x^4.$$

The constant a is 0.01 in our experiments. On the left-hand side, Figure 4.1 shows the solution of the Euler method. The step-size is $h = 0.01$ and the phase portrait is completely incorrect for the chosen starting value $(1.6, 0)$. The solution is turning outwards instead of inwards. In contrast, Figure 4.1 shows the projected Euler method using a larger step-size on the right-hand side. This behaviour for the projected Euler method is to be expected according to Theorem 2.1.

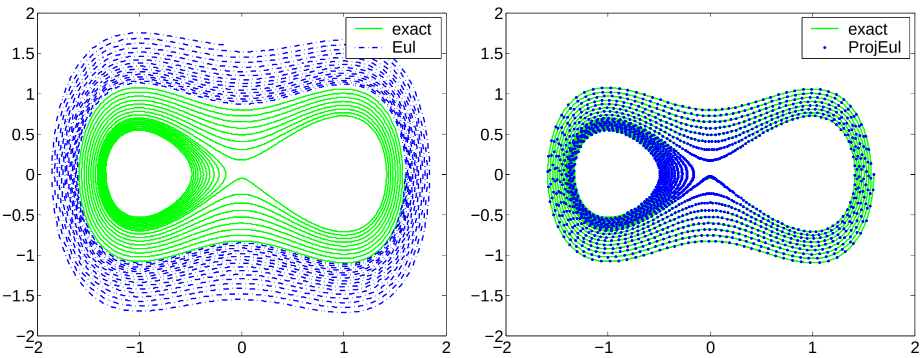

Figure 4.1: Euler method ($h = 0.01$) and projected Euler method ($h = 0.08$)

Besides the projected Euler method we used a third-order Heun method with the Runge-Kutta tableau (cf. [10])

$$\begin{array}{c|ccc} 0 & 0 & & \\ \frac{1}{3} & \frac{1}{3} & & \\ \frac{2}{3} & 0 & \frac{2}{3} & \\ \hline & \frac{1}{4} & 0 & \frac{3}{4} \end{array}$$

That is, the first two steps of the projected method read

Step 1

$$\begin{aligned} g_1 &= y_n \\ g_2 &= y_n + h\tfrac{1}{3}f(g_1) \\ g_3 &= y_n + h\tfrac{2}{3}f(g_2) \\ \tilde{y}_{n+1} &= y_n + h\tfrac{1}{4}f(g_1) + h\tfrac{3}{4}f(g_3) \end{aligned}$$

Step 2

$$V_{n+1} = V(y_n) + h\tfrac{1}{4}\alpha(g_1) + h\tfrac{3}{4}\alpha(g_3)$$

Figure 4.2 shows the solution of the Heun method on the left-hand side. The solution turns inwards but ends up at the wrong equilibrium point. In contrast to this, the projected Heun method (plotted on the right-hand side) with the same step-size already gives the correct solution. This shows that the preservation of the Lyapunov function has a positive effect on the global error. But this is just an observation. An improvement of the global error for the Lyapunov-preserving methods has not been proved in this paper and it is an interesting question for further research.

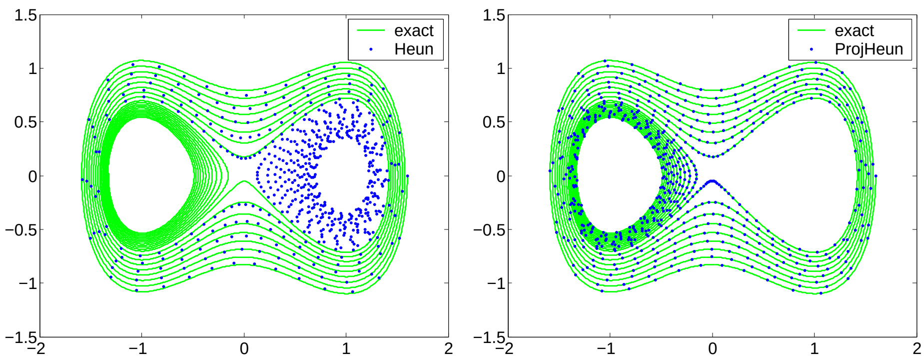

Figure 4.2: Heun method ($h = 0.25$), projected Heun method ($h = 0.25$)

We also tested the symmetric projection methods numerically. Figure 4.3 shows the result for the symmetric projected 2-stage Gauss method.

Figure 4.4 shows that the methods are of the expected order. We use the same starting value as above and numerically compute the solution for a time-span

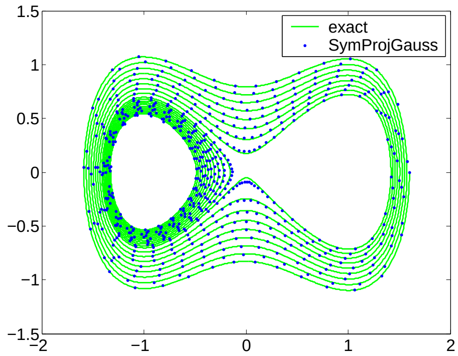

Figure 4.3: Symmetric projected 2-stage Gauss method ($h = 0.25$)

of 1 and different step sizes shown on the x-axis. The result at the endpoint is compared to a standard integrator with step size selection set to high accuracy by using the Euclidean norm. In the logarithmic plot the error is plotted versus the step size. The slopes in this plot indicates the order of the method.

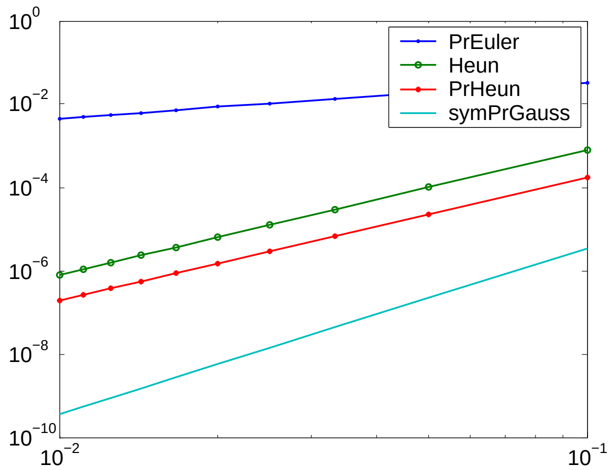

Figure 4.4: Order plot of the projected Euler, Heun, projected Heun and symmetric projected 2-stage Gauss method for the Duffing equation

Finally, we checked the rate of dissipation, that is the approximation of $V(y(t))$. Figure 4.5 shows that the projected Heun method already produces the correct rate of dissipation at a large step size of 0.5, whereas the Heun method without projection indicates a much faster decay.

As a second test equation we used

$$\dot{x} = -y - x(1 - \sqrt{x^2 + y^2})^2$$

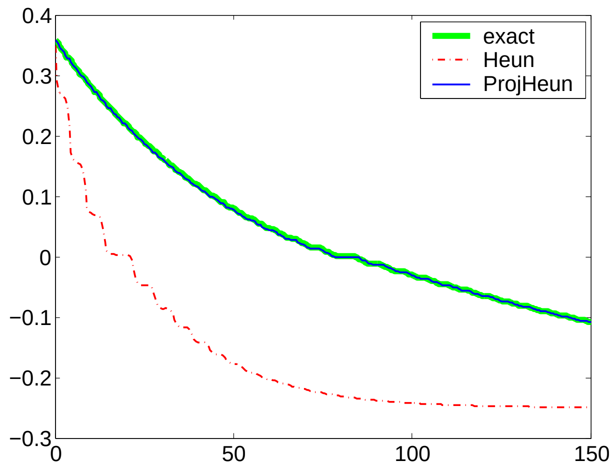

Figure 4.5: Rate of dissipation of the Heun and projected Heun method for the Duffing equation. Step size $h = 0.5$, starting value (1.6, 0) and time=[0, 150].

$$\dot{y} = x - y(1 - \sqrt{x^2 + y^2})^2$$

with the Lyapunov function

$$V(x, y) = x^2 + y^2.$$

The solutions outside the circle are attracted to the circle with radius one and stay there in the exact ordinary differential equation. They are repelled from the circle, if the initial value is within the circle and stay on the circle, if the initial value is on the circle. The starting value $(1.6, 0)$ is chosen in our experiments and we integrated numerically for the time-span [0, 150]. Figure 4.6 shows the results for the Heun method and for the projected Heun method. The Heun method does not properly reflect the expected behaviour. The projected Heun method does a better job in recognising the circle with $\alpha(y) = 0$. Finally, that is by continuing the numerical integration for a longer time, the projected method will also turn in due to round-off error. If a numerical approximation entered the circle once, the correct behaviour of attraction to the origin is observed. The discrete Lyapunov function only guarantees the preservation of stability regions, but the improvement over the unprojected method at the circle with $\alpha(y) = 0$ is significant.

A last experiment concerns the reversing symmetries. We use the gradient system $\dot{y} = -\nabla V(y)$ with the strict Lyapunov function

$$V(x, y) = \frac{1}{\left(\sqrt{(x+1)^2 + y^2} + 1\right)} + \frac{-1}{\left(\sqrt{(x-1)^2 + y^2} + 1\right)}$$

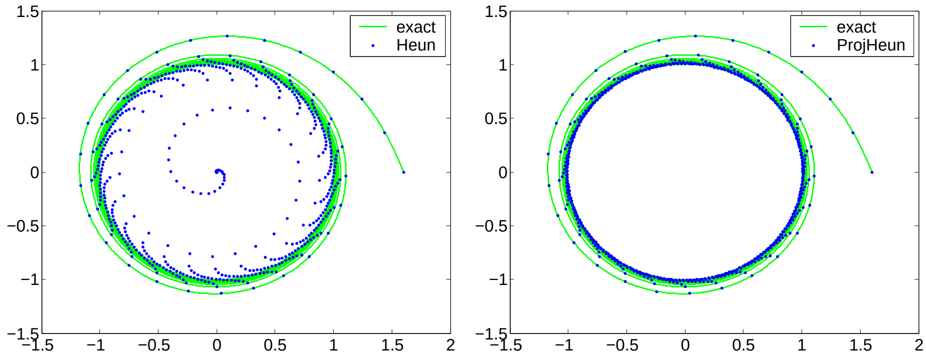

Figure 4.6: Heun method ($h = 0.25$), projected Heun method ($h = 0.25$)

as a test equation. This ODE has the reversing symmetry

$$R\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -x \\ y \end{pmatrix}.$$

This symmetry has the reflection symmetry of the phase portrait with respect to the y-axis as a consequence. To check the preservation of the symmetry, we perform the following experiment. We choose $(x_0, y_0) = (0, 10)$ on the y-axis as initial condition. Then we compute the solution from time $t_0 = 0$ to time $t_1 = 3100$ with step size $h = 0.5$. Then we take the final value y_{6200} and apply the reversing symmetry to get Ry_{6200}. Then we integrate again for a time-span of 3100. According to (3.1), the exact solution arrives at our starting value $(x_0, y_0) = (0, 10)$, due to the reversing symmetry. The result of the numerical integration with the third-order projected Heun method is compared to the result of the second-order symmetric projected one-stage Gauss method in Figure 4.7. The symmetric method that preserves the reversing symmetry is symmetric with respect to the y-axis and returns to the starting value as does the exact solution. The projected Heun method does not preserve the symmetry. The good behaviour of the symmetric projected method is to be expected due to Proposition 3.2.

5 Conclusion

We considered new projection-based methods that preserve an ODE's Lyapunov function as a Lyapunov function for the discrete map given by the numerical method. The approach is flexible enough to be useful in various problems where a Lyapunov function is known. In this article, we only described the basic concepts. The methods can be refined and further adapted to the problem at hand. The symmetric projection methods, which in addition preserve some linear reversing symmetries, are an interesting example for that. Projection has been used to conserve integrals of an ODE. Our approach is a unification in

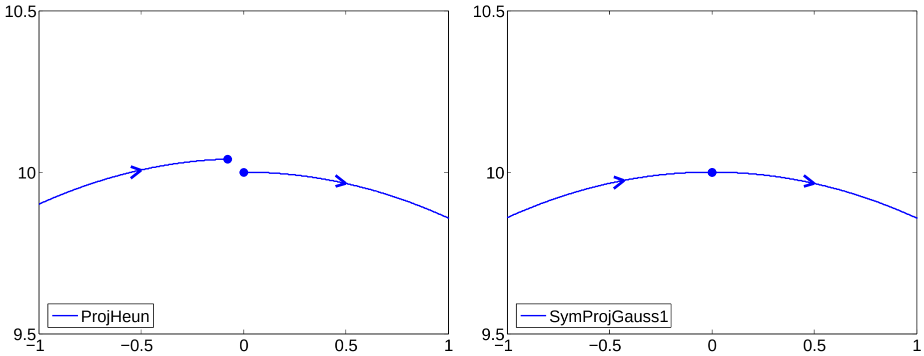

Figure 4.7: Projected Heun method ($h = 0.5$), symmetric projected one-stage Gauss method ($h = 0.5$)

the sense that our methods reduce to integral-preserving methods if V is a first integral. The theoretical results ensure that a nonlinear stability region, given by the Lyapunov function, persists in the numerical methods. The numerical experiments confirm this behaviour but, even more, suggest an overall improvement of the numerical simulation. This occurs especially in regions where $\alpha(y)$ is close to zero as in our second numerical experiment. Hence the theoretical as well as the numerical results are promising and encourage the use of these methods.

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