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Approximation of Hamiltonian Systems using an Alternative Variational Technique

Sergio Amat[1,*], *M. José Legaz*[1] *and Pablo Pedregal*[2]

[1] Departamento de Matemática Aplicada y Estadística, Universidad Politécnica de Cartagena, Spain
[2] E.T.S. Ingenieros Industriales, Universidad de Castilla La Mancha, Campus de Ciudad Real Spain

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Abstract: Hamiltonian systems are related to numerous areas of mathematics and have a lot of application branches, such as classical and quantum mechanics, statistics, optical, astronomy, molecular dynamic, plasma physics, etc. In general, the integration of these systems requires the use of geometric integrators. In this paper, we introduce a new variational approach for models which are formulated naturally as conservative systems of ODEs, most importantly Hamiltonian systems. Our variational method for Hamiltonian systems, which is proposed here, is in some sense symplectic and energy preserving. In addition to introducing the technique, we briefly indicate its most basic properties, and test its numerical performance in some simple examples

Keywords: Hamiltonian systems, symplecticity, energy preserving, variational approach

This paper is dedicated to the memory of Professor José Sousa Ramos.

1 Introduction

It is well-known that numerical methods, such as the ordinary Runge-Kutta schemes, are not particularly efficient in integrating Hamiltonian systems, because Hamiltonian systems are not generic in the set of all dynamic systems. They are not structurally stable against non-Hamiltonian perturbations. Numerical solution of Hamiltonian systems is frequently carried out by symplectic integrators due to their good performance in moderate and long-time integration, see [11,13,16,17, 22]. Symplectic numerical methods belong to the family of Geometric Numerical Integrators, which preserve important qualitative and geometric properties of the underlying differential system, and are arguably the most popular methods in this class. Certain qualitative properties of the evolution, like symplecticity, are preserved and, in general they exhibit smaller error growth along the numerical trajectory.

Some pioneering works on symplectic integrations are due to Vogelaere [26], Ruth [20], and Feng Kang [10]. The derivation of higher-order methods is covered by several approaches such as composition methods, classical Runge-Kutta methods (RK) as well as partitioned Runge-Kutta (PRK) methods, and methods based on generating functions. The systematic study of symplectic Runge-Kutta methods started around 1988, and a complete characterization has been found independently by Lasagni [15] (using the approach of generating functions), and by Sanz-Serna [21] and Suris[24] (using the ideas of the classical papers of Burrage and Butcher [6] and Crouzeix [8] on algebraic stability).

Nowadays, it is well-known that certain implicit RK methods of Radau type (generalizing the implicit Euler method) are useful in the context of systems with strong dissipation, like electronic circuits or chemical reaction dynamics. Partitioned Runge- Kutta (PRK) methods are another way to approximating the solution trajectory which it is based on using different approximation formulas for different components of the solution. (use different sets of quadrature rules for each subset of the variables). The starting point of generating function (GF) theory was the discovery of Hamilton that the motion of the system is completely described by a characteristic function S, and that S is the solution of a partial differential equation, now called the Hamilton-Jacobi differential equation. It was noticed later, especially by

* Corresponding author e-mail: sergio.amat@upct.es

Siegel (Siegel and Moser 1971), that such a function S is directly connected to any symplectic map. It was called generating function. See [11,16].

Another important point should be taken into account regarding Hamiltonian systems, even with symplectic maps, and that is the lack of energy conservation in the map. It would seem to be an obvious goal for Hamiltonian integration methods both to preserve the symplectic structure and to conserve the energy, but it was shown that this was in general impossible. Thus a symplectic map which only approximates a Hamiltonian cannot conserve energy [27]. Recently, some research has been carried out about energy-preserving symplectic methods based on the key tool line integral associated with conservative vector fields, as well as its discrete version. See,[4,5].

In this contribution, we introduce a new variational approach for models which are formulated naturally as conservative systems of ODEs, most importantly Hamiltonian systems. The variational method for Hamiltonian systems, which is proposed here, is in some sense symplectic and energy preserving, and is based on a natural modification of the schemes introduced in [1,2,3]. We perform an initial brief analysis of the approach both theoretically and numerically.

2 A new variational approach for Hamiltonian systems

Consider the hamiltonian dynamical system

$$\mathbf{x}'(t)=\frac{\partial \mathbf{H}}{\partial \mathbf{p}}(\mathbf{x}(t),\mathbf{p}(t)),\quad \mathbf{p}'(t)=-\frac{\partial \mathbf{H}}{\partial \mathbf{x}}(\mathbf{x}(t),\mathbf{p}(t)),\quad (1)$$

to hold in a certain time interval $(0,T)$, subject to initial boundary conditions $(\mathbf{x}(0),\mathbf{p}(0))=(\mathbf{x}_0,\mathbf{p}_0)$. Both $\mathbf{x}$ and $\mathbf{p}$ take on values in $\mathbf{R}^N$. We are interested in setting up a method to understand, and approximate, the trajectories of such a system. In particular, we would like to focus on how the a priori knowledge of conserved quantities may help in improving our ability to approximate such system. It is well-known that the hamiltonian itself $\mathbf{H}(\mathbf{x},\mathbf{p}):\mathbf{R}^N\times\mathbf{R}^N\to\mathbf{R}$ is one such conserved quantity so that $\mathbf{H}(\mathbf{x}(t),\mathbf{p}(t))=\mathbf{H}(\mathbf{x}_0,\mathbf{p}_0)\equiv\mathbf{H}_0$ for all times t in $(0,T)$.

Recently, an alternative to the analysis and numerical approximation of dynamical systems has been introduced ([1,2,3]), based on the minimization of the error functional

$$E(\mathbf{X})=\int_0^T\frac{1}{2}|\mathbf{X}'(t)-\mathbf{F}(\mathbf{X}(t))|^2\,dt$$

regarded as a measure of how far a given absolutely-continuous path $\mathbf{X}$ complying with $\mathbf{X}(0)=\mathbf{X}_0$ is from being a solution of the underlying dynamical system

$$\mathbf{X}'(t)=\mathbf{F}(\mathbf{X}(t))\text{ in }(0,T),\quad \mathbf{X}(0)=\mathbf{X}_0.\quad (2)$$

It is elementary to realize that solutions of the system are precisely those $\mathbf{X}$ for which $E(\mathbf{X})=0$, and preserve the initial condition. We would like to explore one possibility of taking advantage of the hamiltonian structure of the system for this variational approach. Namely, if the dimension is even $2N$, and (1) holds for some hamiltonian $\mathbf{H}$, then, as remarked above, $\mathbf{H}$ must be constant on integral curves, and so we could modify the error functional to take into account this extra information to write

$$E(\mathbf{x},\mathbf{p})=\int_0^T\left[\frac{1}{2}|\mathbf{x}'-\frac{\partial \mathbf{H}}{\partial \mathbf{p}}(\mathbf{x},\mathbf{p})|^2+\frac{1}{2}|\mathbf{p}'+\frac{\partial \mathbf{H}}{\partial \mathbf{x}}(\mathbf{x},\mathbf{p})|^2\right.$$
$$\left.+\frac{1}{2}|\mathbf{H}(\mathbf{x},\mathbf{p})-\mathbf{H}_0|^2\right]dt.\quad (3)$$

The basis for our proposal is the following.

Proposition 1. *Suppose the path* $\mathbf{x}$ *is a critical point for the functional in (3), under the initial condition* $(\mathbf{x}(0),\mathbf{p}(0))=(\mathbf{x}_0,\mathbf{p}_0)$. *Then* $\mathbf{x}$ *is the unique solution of (1).*

Proof:

Since we are assuming that all of our ingredients are sufficiently smooth, we can differentiate as many times as necessary without being concerned about its validity. Hence, it is straightforward to write down the Euler-Lagrange optimality conditions for a critical path of (3) in the form

$$-\left(\mathbf{x}'-\frac{\partial \mathbf{H}}{\partial \mathbf{p}}(\mathbf{x},\mathbf{p})\right)'-\left(\mathbf{x}'-\frac{\partial \mathbf{H}}{\partial \mathbf{p}}(\mathbf{x},\mathbf{p})\right)\frac{\partial^2 \mathbf{H}}{\partial \mathbf{x}\partial \mathbf{p}}(\mathbf{x},\mathbf{p})+$$
$$\left(\mathbf{p}'+\frac{\partial \mathbf{H}}{\partial \mathbf{x}}(\mathbf{x},\mathbf{p})\right)\frac{\partial^2 \mathbf{H}}{\partial \mathbf{x}^2}(\mathbf{x},\mathbf{p})+(\mathbf{H}(\mathbf{x},\mathbf{p})-\mathbf{H}_0)\frac{\partial \mathbf{H}}{\partial \mathbf{x}}(\mathbf{x},\mathbf{p})=0,$$
$$-\left(\mathbf{p}'+\frac{\partial \mathbf{H}}{\partial \mathbf{x}}(\mathbf{x},\mathbf{p})\right)'-\left(\mathbf{x}'-\frac{\partial \mathbf{H}}{\partial \mathbf{p}}(\mathbf{x},\mathbf{p})\right)\frac{\partial^2 \mathbf{H}}{\partial \mathbf{p}^2}(\mathbf{x},\mathbf{p})+$$
$$\left(\mathbf{p}'+\frac{\partial \mathbf{H}}{\partial \mathbf{x}}(\mathbf{x},\mathbf{p})\right)\frac{\partial^2 \mathbf{H}}{\partial \mathbf{x}\partial \mathbf{p}}(\mathbf{x},\mathbf{p})+(\mathbf{H}(\mathbf{x},\mathbf{p})-\mathbf{H}_0)\frac{\partial \mathbf{H}}{\partial \mathbf{p}}(\mathbf{x},\mathbf{p})=0.$$

In addition, we also have the transversality or natural condition at the end-point $t=T$,

$$\mathbf{x}'-\frac{\partial \mathbf{H}}{\partial \mathbf{p}}(\mathbf{x},\mathbf{p})\Big|_{t=T}=\mathbf{p}'+\frac{\partial \mathbf{H}}{\partial \mathbf{x}}(\mathbf{x},\mathbf{p})\Big|_{t=T}=\mathbf{0}.$$

If we put

$$\mathbf{X}=\mathbf{x}'-\frac{\partial \mathbf{H}}{\partial \mathbf{p}}(\mathbf{x},\mathbf{p}),\quad \mathbf{P}=\mathbf{p}'+\frac{\partial \mathbf{H}}{\partial \mathbf{x}}(\mathbf{x},\mathbf{p}),\quad (4)$$

we can rewrite the above big system in the form

$$\mathbf{X}'+\mathbf{X}\frac{\partial^2 \mathbf{H}}{\partial \mathbf{x}\partial \mathbf{p}}(\mathbf{x},\mathbf{p})-\mathbf{P}\frac{\partial^2 \mathbf{H}}{\partial \mathbf{x}^2}(\mathbf{x},\mathbf{p})=(\mathbf{H}(\mathbf{x},\mathbf{p})-\mathbf{H}_0)\frac{\partial \mathbf{H}}{\partial \mathbf{x}}(\mathbf{x},\mathbf{p}),$$
$$\mathbf{P}'+\mathbf{X}\frac{\partial^2 \mathbf{H}}{\partial \mathbf{p}^2}(\mathbf{x},\mathbf{p})-\mathbf{P}\frac{\partial^2 \mathbf{H}}{\partial \mathbf{x}\partial \mathbf{p}}(\mathbf{x},\mathbf{p})=(\mathbf{H}(\mathbf{x},\mathbf{p})-\mathbf{H}_0)\frac{\partial \mathbf{H}}{\partial \mathbf{p}}(\mathbf{x},\mathbf{p}).$$

We also have that $\mathbf{X}(T)=\mathbf{P}(T)=\mathbf{0}$. We would like to conclude that the only pair complying with these

conditions is $\mathbf{X} \equiv \mathbf{0}$, $\mathbf{P} \equiv \mathbf{0}$. Note that this would be immediate, if in the error functional in (3) there is no term about the conservation of the energy, for in this case the problem for the pair $(\mathbf{X},\mathbf{P})$ would be

$$\mathbf{X}' + \mathbf{X}\frac{\partial^2 \mathbf{H}}{\partial \mathbf{x}\partial \mathbf{p}}(\mathbf{x},\mathbf{p}) - \mathbf{P}\frac{\partial^2 \mathbf{H}}{\partial \mathbf{x}^2}(\mathbf{x},\mathbf{p}) = \mathbf{0},$$
$$\mathbf{P}' + \mathbf{X}\frac{\partial^2 \mathbf{H}}{\partial \mathbf{p}^2}(\mathbf{x},\mathbf{p}) - \mathbf{P}\frac{\partial^2 \mathbf{H}}{\partial \mathbf{x}\partial \mathbf{p}}(\mathbf{x},\mathbf{p}) = \mathbf{0},$$

together with $\mathbf{X}(T) = \mathbf{P}(T) = \mathbf{0}$. The unique solution is $\mathbf{X} \equiv 0, \mathbf{P} \equiv 0$. This was the general point of view adopted in earlier contributions by the authors ([1,2,3]) for a general-purpose procedure. We want to conclude that it is also so even with the added energy term

$$\int_0^T \frac{1}{2}|\mathbf{H}(\mathbf{x},\mathbf{p}) - \mathbf{H}_0|^2\, dt$$

to the error functional. The whole point of our concern here is to assess how this extra term on the conservation of energy may affect the numerical performance of the underlying numerical scheme.

To show our aim, we define the mapping $(\tilde{\mathbf{x}},\tilde{\mathbf{p}}) = \mathscr{T}(\mathbf{x},\mathbf{p})$ as follows: given $(\mathbf{x},\mathbf{p})$, solve the linear system for $(\mathbf{X},\mathbf{P})$ above under the final time condition $\mathbf{X}(T) = \mathbf{P}(T) = \mathbf{0}$; once $(\mathbf{X},\mathbf{P})$ is known, let $(\tilde{\mathbf{x}},\tilde{\mathbf{p}})$ be the solution of (4) under the initial condition $\tilde{\mathbf{x}}(0) = \mathbf{x}_0$, $\tilde{\mathbf{p}}(0) = \mathbf{p}_0$. The true solution of (1) is certainly a fixed point for this mapping $\mathscr{T}$. We claim that it is the only such fixed point. If this is so, our proposition is proved.

As indicated, our mapping $\mathscr{T}$ is the composition of two operations. The first one is the passage $(\mathbf{x},\mathbf{p}) \mapsto (\mathbf{X},\mathbf{P})$ through

$$\begin{pmatrix}\mathbf{X}\\ \mathbf{P}\end{pmatrix}' = \mathbf{A}(\mathbf{x},\mathbf{p})\begin{pmatrix}\mathbf{X}\\ \mathbf{P}\end{pmatrix} + \mathbf{b}(\mathbf{x},\mathbf{p}) \text{ in } (0,T),$$
$$(\mathbf{X}(T),\mathbf{P}(T)) = \mathbf{0},$$

where the matrix $\mathbf{A}$ depends on second derivatives of $\mathbf{H}$ evaluated at $(\mathbf{x},\mathbf{p})$, and $\mathbf{b}$ depends on $\mathbf{H}$, and its first derivatives. If we now have two pairs $(\mathbf{x}_i,\mathbf{p}_i)$, $i = 1,2$, then a standard application of Gronwall's lemma lead to

$$\|(\mathbf{X}_1,\mathbf{P}_1) - (\mathbf{X}_2,\mathbf{P}_2)\| \le MT\|(\mathbf{x}_1,\mathbf{p}_1) - (\mathbf{x}_2,\mathbf{p}_2)\|$$

where the constant M comes from the Lipstchitz constants for $\mathbf{H}$, and its derivatives. By taking T sufficiently small the transformation $(\mathbf{x},\mathbf{p}) \mapsto (\mathbf{X},\mathbf{P})$ is a contraction. The second operation can be treated similarly.

We conclude that our mapping $\mathscr{T}$, for small T, is a contraction, and can only admit a unique fixed point, which has to be the solution of (1). This argument can be used successively in small time intervals to cover any finite interval in a finite number of steps.

□

What Proposition 1 ensures is that the only critical points of the error functional (3) are the solutions of the hamiltonian system (1) itself, and so an approximation procedure based on minimizing the error functional can never get stuck in local minima, but proceed to steadily approximate the true solution of the dynamical system. Moreover, by construction, the functional penalizes the non conservation of the energy.

3 A steepest descent direction for our functional

We focus on finding the steepest descent direction with respect to the norm

$$\int_0^T |\mathbf{Y}'(t)|^2 dt,$$

in this case, the steepest descent direction can be found as the solution of a variational problem of the following form.

Minimize $\mathbf{Y}$:

$$\frac{1}{2}\int_0^T [|\mathbf{Y}'|^2 + (\mathbf{X}' - \Omega\nabla\mathbf{H}(\mathbf{X})(\mathbf{Y}' + \Omega^T\nabla^2\mathbf{H}(\mathbf{X})\mathbf{Y})$$
$$+(\mathbf{H}(\mathbf{X}) - \mathbf{H}(\mathbf{X}(0)))\nabla\mathbf{H}(\mathbf{X})\mathbf{Y}]\, dt,$$

under $\mathbf{Y}(0) = 0$, where

$$\Omega = \begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}. \tag{5}$$

This is a standard quadratic variational problem whose optimal solution can be found through the system

$$-\frac{d}{dt}\left[\mathbf{Y}' + \mathbf{X}' + \Omega^T\nabla\mathbf{H}(\mathbf{X})\right]$$
$$+\nabla^2\mathbf{H}(\mathbf{X})\Omega\left(\mathbf{X}' + \Omega^T\nabla\mathbf{H}(\mathbf{X})\right) + (\mathbf{H}(\mathbf{X}) - \mathbf{H}(\mathbf{X}_0))\nabla\mathbf{H}(\mathbf{X}) = 0$$

in $(0,T)$, together with the end-point conditions

$$\mathbf{Y}(0) = 0, \mathbf{Y}'(T) + \mathbf{X}'(T) + \Omega^T\nabla\mathbf{H}(\mathbf{X}(T)) = 0.$$

It is remarkable that the solution of this system can be given in an fully explicit form as

$$\mathbf{Y}(t) = -\int_0^t [s\mathbf{G}(s) + \mathbf{F}(s)]\, ds - t\int_t^T \mathbf{G}(s)\, ds, \tag{6}$$

where

$$\mathbf{F} = \mathbf{X}' + \Omega^T\nabla\mathbf{H}(\mathbf{X})$$
$$\mathbf{G} = \nabla^2\mathbf{H}(\mathbf{X})\Omega(\mathbf{X}' + \Omega^T\nabla\mathbf{H}(\mathbf{X})) + (\mathbf{H}(\mathbf{X}) - \mathbf{H}(\mathbf{X}(0)))\nabla\mathbf{H}(\mathbf{X}).$$

We can therefore establish a steepest descent strategy to decrease the error in each iteration. Note that the derivative of the error at $\mathbf{X}$ in the direction $\mathbf{Y}$ is

$$-\int_0^T |\mathbf{Y}'(t)|^2 dt$$

Then we can choose $\eta \in (0,1)$ such that

$$E(\mathbf{X}+\eta\mathbf{Y}) \leq E(\mathbf{X}) - \frac{1}{2}\int_0^T |\mathbf{Y}'(t)|^2 dt.$$

Moreover, it is possible to check uniform convergence of this procedure for smooth Hamiltonian systems (see [18]). The following statement is a direct adaptation of similar results in [18].

Theorem 1. *The iterative procedure* $\mathbf{X}^{(j)} = \mathbf{X}^{(j-1)} + \eta_j \mathbf{Y}^{(j)}$, *starting from arbitrary feasible* $\mathbf{X}^{(0)}$, *converges strongly in* $H^1(0,T)$ *to the unique solution of any sufficiently smooth Hamiltonian system.*

4 Numerical results

The iterative numerical procedure is easily implementable.

1. Start with an initial approximation $\mathbf{X}^0(t)$ compatible with the initial conditions, for instance $\mathbf{X}^{(0)}(t) = \mathbf{X}_0$.
2. Assume we have approximation $(\mathbf{X}^{(j)})(t)$ in $[0,T]$.
3. Compute its derivative $(\mathbf{X}^{(j)})'(t)$.
4. Define $\mathbf{F}$ and $\mathbf{G}$ through the formulas

$$\mathbf{F}^{(j)} = (\mathbf{X}^{(j)})' + \Omega^T \nabla \mathbf{H}(\mathbf{X}^{(j)}),$$
$$\mathbf{G}^{(j)} = \nabla^2 \mathbf{H}(\mathbf{X}^{(j)})\Omega((\mathbf{X}^{(j)})' + \Omega^T \nabla \mathbf{H}(\mathbf{X}^{(j)})) + (\mathbf{H}(\mathbf{X}^{(j)}) - \mathbf{H}(\mathbf{X}(0)))\nabla \mathbf{H}(\mathbf{X}^{(j)}).$$

5. Approximate the mapping

$$\mathbf{Y}^{(j)}(t) = -\int_0^t \left[s\mathbf{G}^{(j)}(s) + \mathbf{F}^{(j)}(s)\right] ds - t\int_t^T \mathbf{G}^{(j)}(s)\, ds, \tag{7}$$

using (symplectic) quadrature formulas.

6. Update $\mathbf{X}^{(j)}$ to $\mathbf{X}^{(j+1)}$ by using the formula

$$\mathbf{X}^{(j+1)}(t) = \mathbf{X}^{(j)}(t) + \eta_j \mathbf{Y}^{(j)}(t).$$

7. Iterate (3), (4), (5) and (6) until numerical convergence.

We test this numerical procedure with two classical systems: a Lotka-Volterra problem, and the Kepler problem. In particular, we would like to stress the necessity of using symplectic rules for the approximation of $\mathbf{Y}^{(j)}$.

The Lotka-Volterra problem can be given in normal form

$$\begin{aligned} p' &= e^q - 2, \\ q' &= 1 - e^p. \end{aligned} \tag{8}$$

The initial conditions considered are $p = 2.3$ and $q = 0.7$.

It is well known that this Lotka-Volterra problem is defined as two species problem: one is a predator, the other one its prey. It is frequently used to describe the dynamics of biological systems, in which two species interact.

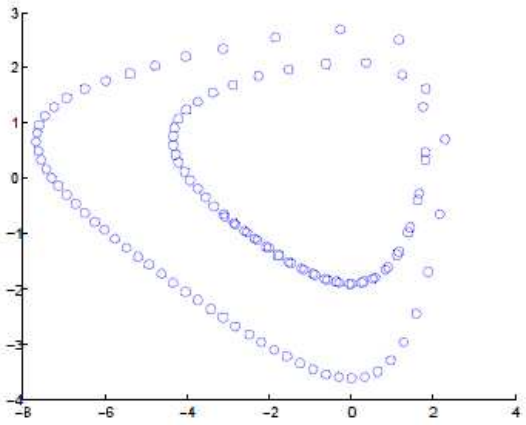

Fig. 1: The q-coordinate versus p-coordinate,'o'-approximation. Problem 8 using the non symplectic trapezoidal rule.

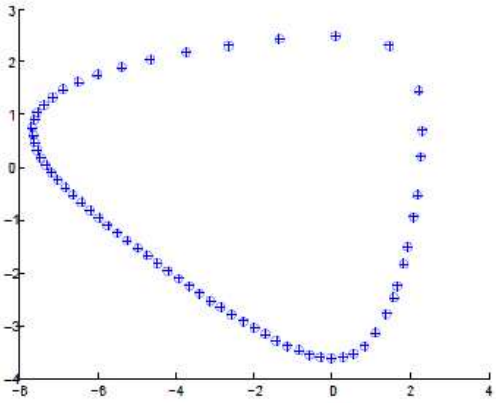

Fig. 2: The x-coordinate versus y-coordinate,'o'-original,'+'-approximation. Problem 8 using the symplectic mid-point quadrature rule.

The Kepler problem can be stated as

$$\begin{aligned} p_i' &= -\frac{q_1}{(q_1^2+q_2^2)^{\frac{3}{2}}}, \\ q_i' &= p_i. \end{aligned} \tag{9}$$

for $i = 1,2$. The initial conditions have been taken to be $p_1 = 0.4$, $p_2 = 0$, $q_1 = 0$ and $q_2 = 2$.

The Kepler problem in classical mechanics is a special case of the two-body problem, in which two bodies interact

through a central force that varies in strength as the inverse square of the distance between them.

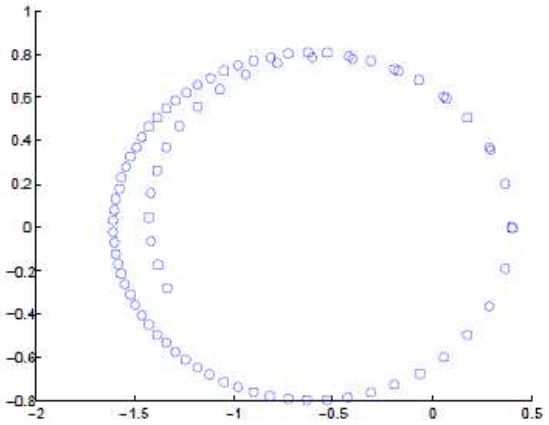

Fig. 3: The q-coordinate versus p-coordinate,'o'-approximation. Problem 9 using the non symplectic trapezoidal rule.

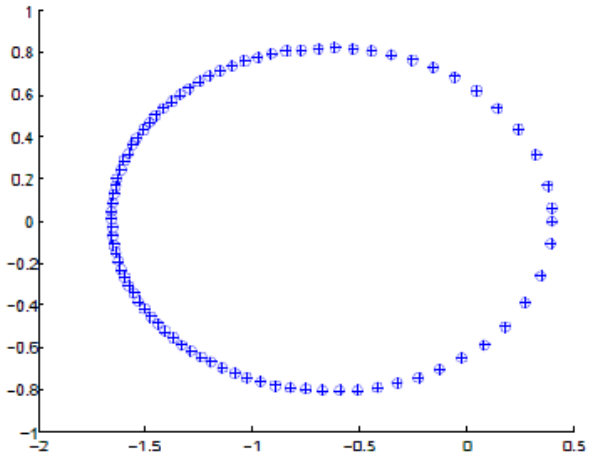

Fig. 4: The x-coordinate versus y-coordinate,'o'-original,'+'-approximation. Problem 9 using the symplectic mid-point quadrature rule.

The approximations using the non symplectic trapezoidal rule are not satisfactory, see Figures 1 and 3. This situation can be resolved by considering other types of quadrature rules, like the family of simplectic ones, to approximate the direction $\mathbf{Y}^{(j)}$ for each iteration step. The good results in Figures 2-4 have been obtained by using mid-point quadrature rule, the simplest symplectic quadrature rule.

5 Concluding remarks

One main point we would like to emphasize is the importance of selecting the descent direction $\mathbf{Y}$ with respect to the norm

$$\int_0^T |\mathbf{Y}'(t)|^2 dt,$$

since in this case we are able to write down $\mathbf{Y}$ in an integral closed form. In this situation, we can use very well known symplectic quadrature rules. In other cases, we would need to approximate the resulting second order boundary-value problem using symplectic methods. This possibility still deserves some attention. Nevertheless, recently, a symplectic algorithm based on the dual variational principle has been proposed for solving the nonlinear two-point boundary value problem [19].

Finally, we would like to highlight the advantages of our approach.

- –A symplectic map which only approximates a Hamiltonian cannot conserve energy [27]. In our case, by definition the functional penalizes the nonpreservation of the energy, and our linearization can be approximated by well known sympletic quadrature rules. In fact, for polynomial systems, the formula for the direction $\mathbf{Y}$ can be obtained exactly.
- –In the non-stiff situation, the long-time behaviour of symplectic methods is well understood, and can be explained with the help of a backward error analysis (modified equations). In the highly oscillatory (stiff) case, this theory breaks down. However, our base linearization is well understood in both cases.

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Sergio Amat received the M.S., B.S., and Ph.D. degrees in mathematics from Universidad de Valencia, Valencia, Spain, in 1996 and 2001, respectively. Currently, he is Full Professor in the Department of Applied Mathematics and Statistics, Universidad Politécnica de Cartagena, Cartagena, Spain. His research interests include nonlinear reconstructions, multiresolution and wavelets algorithms, as well as iterative schemes for nonlinear equations and numerical approximation of differential equations.

M. J. Legaz received the M.S. and B.S. degrees in Naval Architecture and Ocean Engineer from the Universidad Politécnica de Cartagena, Cartagena, Spain, in 2008. Currently, she is a PhD student in the Department of Applied Mathematics and Statistics of the Universidad Politécnica de Cartagena. Her research interests include the numerical approximation of nonlinear and differential equations.

Pablo Pedregal received the PhD degree in Applied Mathematics in the University of Minnesota. His research interests are in the areas of applied mathematics, particularly optimization understood in a broad sense. He has published research articles in reputed international journals of applied mathematics and analysis. He is referee and editor of mathematical journals.