Adjoint-based exact Hessian-vector multiplication using symplectic Runge–Kutta methods

Shin-ichi Ito · Takeru Matsuda · Yuto Miyatake

Received: date / Accepted: date

Abstract We consider a function of the numerical solution of an initial value problem, its Hessian matrix with respect to the initial data, and the computation of a Hessian-vector multiplication. A simple way of approximating the Hessian-vector multiplication is to integrate the so-called second-order adjoint system numerically. However, the error in the approximation could be significant unless the numerical integration is sufficiently accurate. This paper presents a novel algorithm that computes the intended Hessian-vector multiplication exactly. For this aim, we give a new concise derivation of the second-order adjoint system and show that the intended multiplication can be computed exactly by applying a particular numerical method to the second-order adjoint system. In the discussion, symplectic partitioned Runge–Kutta methods play an important role.

Keywords Hessian · adjoint method · symplectic partitioned Runge–Kutta method

Mathematics Subject Classification (2010) 34H05 · 65F10 · 65K10 · 65L05 · 65L06 · 65P10

S. Ito
Earthquake Research Institute, The University of Tokyo
E-mail: ito@eri.u-tokyo.ac.jp

T. Matsuda
Department of Mathematical Informatics, Graduate School of Information Science and Technology, The University of Tokyo
E-mail: matsuda@mist.i.u-tokyo.ac.jp

Y. Miyatake
Cybermedia Center, Osaka University, Osaka, Japan
E-mail: miyatake@cas.cmc.osaka-u.ac.jp
1 Introduction

We consider a system of ordinary differential equations (ODEs) of the form
\[
\frac{dx(t; \theta)}{dt} = f(x(t; \theta)), \quad x(0) = \theta,
\] (1.1)
where \( f : \mathbb{R}^d \to \mathbb{R}^d \) is assumed to be sufficiently differentiable, and \( \theta \) is an initial data. ODEs are often solved numerically, and we denote the numerical solutions by \( x_n(\theta) \approx x(t_n; \theta) = x(nh; \theta) \), where \( h \) is the time step size. Let \( C : \mathbb{R}^d \to \mathbb{R} \) be a twice differentiable function. We are concerned with numerical computation of the gradient \( \nabla_\theta C(x_N(\theta)) \) and Hessian \( H_\theta C(x_N(\theta)) \) of the function \( C \) with respect to the initial data \( \theta \).

Calculating the gradient vector \( \nabla_\theta C(x_N(\theta)) \) is often required when we solve the optimization problem
\[
\min_\theta C(x_N(\theta)).
\]
One simple way of obtaining an approximation to the gradient is to integrate the system (1.1) numerically multiple times for perturbed initial data. For example
\[
\frac{C(x_N(\theta + \Delta e_i)) - C(x_N(\theta))}{\Delta},
\] (1.2)
where \( \Delta \) is a small scalar constant and \( e_i \) is the \( i \)-th column of the \( d \)-dimensional identity matrix, can be seen as an approximation to the \( i \)-th component of the gradient. However, when the dimensionality \( d \) or the number of time steps \( N \) is large, this approach becomes computationally expensive, which makes it difficult to obtain a sufficiently accurate approximation. Instead, in various fields such as optimal design in aerodynamics [4], variational data assimilation in meteorology and oceanography [2], and inversion problems in seismology [3], the adjoint method has been used to approximate the gradient: the gradient is approximated by integrating the so-called adjoint system numerically. This approach is more efficient than the simple approach in most cases, but the accuracy of the approximation is still limited when there are highly collected discretization errors. More recently, Sanz-Serna [7] showed that, if \( x_N(\theta) \) is the solution of a Runge–Kutta method, the gradient \( \nabla_\theta C(x_N(\theta)) \) can be calculated exactly by solving the adjoint system with a particular choice of Runge–Kutta method.

Hessian matrices also arise in several contexts. For example, if we apply the Newton method to the problem (1.2), a linear system whose coefficient matrix is the Hessian with respect to the initial data \( \theta \) needs to be solved. Further, the information of the inverse of the Hessian is used to quantify the uncertainty for the estimation in the Bayesian context [6, 11]. This case also requires solving a linear system whose coefficient matrix is the Hessian to calculate the inverse.

There are, however, several difficulties in solving such a linear system numerically. As is the case with the gradient, the simplest way of obtaining all elements of the Hessian is to integrate the system (1.1) multiple times for perturbed initial data. However, this approach is noticeably expensive, and further may suffer from
the discretization error. Therefore, calculating all elements of the Hessian by this simple approach is often computationally prohibitive. If we apply a Krylov subspace method such as the conjugate gradient method, there is no need to have full entries of the Hessian, and instead, all we need to do is to compute a Hessian-vector multiplication, i.e. \((H_\theta C(x_N(\theta)))\gamma\) for a given vector \(\gamma \in \mathbb{R}^d\). It was pointed out in \([12, 13]\) that, if \(C\) is a function of the exact solution to (1.1), the Hessian-vector multiplication \((H_\theta C(x(t_N; \theta)))\gamma\) can be obtained by solving the so-called second-order adjoint system backwardly. This property indicates that solving the second-order adjoint system numerically gives an approximation to the intended Hessian-vector multiplication \((H_\theta C(x_N(\theta)))\gamma\). However, when the numerical solutions to the original system (1.1) or second-order adjoint system are not sufficiently accurate, the error between the intended Hessian-vector multiplication \((H_\theta C(x_N(\theta)))\gamma\) and its approximation could be substantial.

In this paper, we extend the aforementioned technique, which was proposed by Sanz-Serna \([7]\) to get the exact gradient, to calculate the exact Hessian-vector multiplication. More precisely, focusing on Runge–Kutta methods and their numerical solutions, we shall propose an algorithm that computes the Hessian-vector multiplication \((H_\theta C(x_N(\theta)))\gamma\) exactly. For this aim, we give a new concise derivation of the second-order adjoint system, which makes it possible to discuss the second-order adjoint system within the framework of the conventional (first-order) adjoint system and to apply the technique \([7]\) to the second-order adjoint system. We show that the intended Hessian-vector multiplication can be calculated by applying a particular choice of Runge–Kutta method to the second-order adjoint system.

In Section 2, we give a brief review of adjoint systems and the paper by Sanz-Serna \([7]\). The main results are shown in Section 3, where we present a new concise derivation of the second-order adjoint system, show how to compute the intended Hessian-vector multiplication exactly, and verify the exactness by a numerical experiment for a small toy problem.

## 2 Preliminaries

In this section, we give a brief review of adjoint systems and the paper by Sanz-Serna \([7]\). In Section 2.1, we focus on the continuous case, where \(C\) is a function of the exact solution to (1.1), and explain how the gradient \(V_\theta C(x(t_N; \theta))\) and the Hessian-vector multiplication \((H_\theta C(x(t_N; \theta)))\gamma\) are obtained based on the adjoint system and second-order adjoint system, respectively. In Section 2.2, we explain that the gradient \(V_\theta C(x_N(\theta))\) can be calculated by solving the adjoint system using a particular choice of Runge–Kutta method.

### 2.1 Adjoint method

Let \(\pi(t)\) be the solution to (1.1) for the perturbed initial condition \(\pi(0) = \theta + \epsilon\). By linearizing the system (1.1) at \(x(t)\), we see that as \(\|\epsilon\| \to 0\) it follows that \(\pi(t) = \)
\[ x(t) + \delta(t) + o(\|\epsilon\|) \], where \( \delta(t) \) solves the variational system
\[
\frac{d}{dt} \delta = \nabla_x f(x) \delta. \tag{2.1}
\]
The adjoint system of (2.1), which is usually introduced by using Lagrange multipliers, is given by
\[
\frac{d}{dt} \lambda = -\nabla_x f(x)^\top \lambda. \tag{2.2}
\]
For the solutions to (2.1) and (2.2), \( \delta(t) \) is constant because
\[
\frac{d}{dt} \lambda(t) \delta(t) = \left( \frac{d}{dt} \lambda(t) \right) \delta(t) + \lambda(t) \left( \frac{d}{dt} \delta(t) \right) = 0.
\]
Thus, we have \( \lambda(t_N)^\top \delta(t_N) = \lambda(0)^\top \delta(0) \), which indicates that
\[
\nabla_x C(x(t_N; \theta))^\top \delta(t_N) = \nabla_\theta C(x(t_N; \theta))^\top \delta(0)
\]
for any \( \delta(0) \), because of the chain rule
\[
\nabla_\theta C(x(t_N; \theta)) = \nabla_\theta x(t_N; \theta)^\top \nabla_x C(x(t_N; \theta))
\]
and
\[
\delta(t) = (\nabla_\theta x(t; \theta)) \delta(0).
\]
It is thus concluded that solving the adjoint system (2.2) backwardly with the final state \( \lambda(t_N) = \nabla_x C(x(t_N; \theta)) \) leads to the intended gradient at \( t = 0 \), i.e. \( \lambda(0) = \nabla_\theta C(x(t_N; \theta)) \).

The second-order adjoint system reads \[12, 13\]
\[
\frac{d}{dt} \xi = -\nabla_x f(x)^\top \xi - (\nabla_x (\nabla_x f(x)) \delta)^\top \lambda, \tag{2.3}
\]
where \( \delta(t) \) is the solution to the variational system (2.1) and \( \lambda(t) \) is the solution to the adjoint system (2.2). In [13], the second-order adjoint system is introduced as the variational system of the adjoint system (2.2). Suppose that the initial state for (2.1) is \( \delta(0) = \gamma \) and the final state for (2.2) is \( \lambda(t_N) = \nabla_x C(x(t_N; \theta)) \). Then, solving the second-order adjoint system (2.3) with the final state \( \xi(t_N) = (\nabla_x C(x(t_N; \theta))) \delta(t_N) \) gives the intended Hessian-vector multiplication at \( t = 0 \), i.e. \( \xi(0) = (\nabla_\theta C(x(t_N; \theta))) \gamma \). We here skip the original proof of [12] and shall explain this property based on a new derivation of the second-order adjoint system in Section 3.
2.2 Exact gradient calculation

We consider the discrete case, where $C$ is a function of the numerical solution to (1.1) obtained by a Runge–Kutta method. Sanz-Serna [7] showed that the gradient $\nabla_\theta C(x_N(\theta))$ can be computed exactly by applying a particular choice of Runge–Kutta method for the adjoint system (2.2). We briefly review the procedure.

Assume that the original system (1.1) is discretized by an $s$-stage Runge–Kutta method

$$x_{n+1} = x_n + h \sum_{i=1}^s b_i k_{n,i},$$

$$k_{n,i} = f(X_{n,i}), \quad i = 1, \ldots, s,$$

$$X_{n,i} = x_n + h \sum_{j=1}^s a_{ij} k_{n,j}, \quad i = 1, \ldots, s.$$

We discretize the adjoint system (2.2) with another $s$-stage Runge–Kutta method

$$\lambda_{n+1} = \lambda_n + h \sum_{i=1}^s B_i l_{n,i},$$

$$l_{n,i} = -\nabla_x f(X_{n,i})^\top \Lambda_{n,i}, \quad i = 1, \ldots, s,$$

$$\Lambda_{n,i} = \lambda_n + h \sum_{j=1}^s A_{ij} l_{n,j}, \quad i = 1, \ldots, s.$$

In the continuous case, the adjoint system gives the gradient $\nabla_\theta C(x(t_N; \theta))$ due to the property $\lambda'(t_N) \delta(t_N) = \lambda(0) \delta(0)$. Therefore, in the discrete case, to obtain the exact gradient $\nabla_\theta C(x_N(\theta))$, the numerical solution to the adjoint system must satisfy $\lambda_{n+1}^\top \delta_{n+1} = \lambda_0^\top \delta_0$. In [7], it is proved that if the Runge–Kutta method for the adjoint system is chosen such that the pair of the Runge–Kutta methods for the original system and adjoint system constitute a symplectic partitioned Runge–Kutta method, the property $\lambda_{n+1}^\top \delta_{n+1} = \lambda_0^\top \delta_0$ is guaranteed and the gradient $\nabla_\theta C(x_N(\theta))$ is exactly obtained as shown in Theorem 2.1. We note that the symplecticity is a fundamental concept in numerical analysis for ODEs, and symplectic numerical methods are well known in the context of geometric numerical integration. For more details, we refer the reader to [5] Chapter VI (for symplectic partitioned Runge–Kutta methods, see also [19]).

**Theorem 2.1** ([7]) Assume that the coefficients $A_{ij}$ and $B_i$ of the Runge–Kutta method for the adjoint system (2.2) satisfy the relation

$$b_i = B_i, \quad i = 1, \ldots, s,$$

$$b_i A_{ij} + B_j a_{ji} = b_i B_j, \quad i, j = 1, \ldots, s.$$

Then, solving the adjoint system with $\lambda_{n+1} = \lambda(t_N) = \nabla_x C(x_N(\theta))$ gives the exact gradient at $n = 0$, i.e. $\lambda_0 = \nabla_\theta C(x_N(\theta))$. 
Remark 2.1  The conditions in Theorem 2.1 indicate that
\[ A_{ij} = b_j - b_j a_{ji}, \]
which makes sense only when every weight \( b_i \) is nonzero. However, for some Runge–Kutta methods such as the Runge–Kutta–Fehlberg method one or more weights \( b_i \) vanish. For such cases, the above conditions cannot be used to find an appropriate Runge–Kutta method for the adjoint system. We refer the reader to Appendix in [7] for a workaround. For clarity, in this paper, we always assume that every weight \( b_i \) is nonzero.

3 Hessian-vector multiplication

Given an arbitrary vector \( \gamma \), we are interested in calculating the Hessian-vector multiplication \((H_{\theta}C(x_N(\theta))))\gamma\) exactly.

In Section 3.1, we give a new concise derivation of the second-order adjoint system (3.1). The idea of the derivation plays an important role in Section 3.2, where we show how to calculate the exact Hessian-vector multiplication \((H_{\theta}C(x_N(\theta))))\gamma\).

3.1 Concise derivation of the second-order adjoint system

Let us couple the original system (1.1) and the variational system (2.1). This leads to the following system
\[
\frac{d}{dt} [x, \delta] = \begin{bmatrix} f(x) \\ \nabla_x f(x) \delta \end{bmatrix}, \quad \begin{bmatrix} x(0) \\ \delta(0) \end{bmatrix} = \begin{bmatrix} \theta \\ \gamma \end{bmatrix}.
\]

If we denote \([x^\top, \delta^\top]^\top\) by \(y\), then (3.1) is written as \(\frac{dy}{dt} = g(y)\). The adjoint system for (3.1) is given by \(\frac{dz}{dt} = -\nabla_y g(y)^\top z\), which can also be written as
\[
\frac{d}{dt} \begin{bmatrix} \xi \\ \lambda \end{bmatrix} = -\begin{bmatrix} \nabla_x f(x)^\top (\nabla_x (\nabla_x f(x) \delta)^\top) \\ 0 \\ \nabla_x f(x)^\top \end{bmatrix} \begin{bmatrix} \xi \\ \lambda \end{bmatrix},
\]

where \(z = [\xi^\top, \lambda^\top]^\top\). Note that the system (3.2) is the combination of the second-order adjoint system (2.3) and the adjoint system (2.2).

As explained in Section 2.1, the Hessian-vector multiplication \((H_{\theta}C(x_N(\theta))))\gamma\) is obtained by solving the second-order adjoint system (2.3) backwardly. This property was proved in Theorem 2 in [12], but we give another proof building on (3.2).

Proposition 3.1  Let \( x, \delta \) and \( \lambda \) be the solutions to the original system (1.1) with the initial state \( x(0) = \theta \), to the variational system (2.1) with the initial state \( \delta(0) = \gamma \) and to the adjoint system (2.2) with the final state \( \lambda(t_N) = \nabla_x C(x(t_N; \theta)) \), respectively.

For the solution to the second-order adjoint system (2.3) with the final state \( \xi(t_N) = (H_{\theta}C(x(t_N; \theta)))\delta(t_N) \), it follows that \(\xi(0) = (H_{\theta}C(x(t_N; \theta))))\gamma\).
Proof Let $\tilde{C} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ be a real valued function defined by
\[
\tilde{C}(x(t_N; \theta), \delta(t_N; \theta)) = \nabla_x C(x(t_N; \theta))^\top \delta(t_N; \theta).
\]
Because
\[
\nabla_\theta C(x(t_N; \theta)) = \nabla_\theta x(t_N; \theta)^\top \nabla_x C(x(t_N; \theta))
\]
and
\[
\delta(t_N; \theta) = \nabla_\theta x(t_N; \theta) \gamma,
\]
the function $\tilde{C}$ can also be written as
\[
\tilde{C}(x(t_N; \theta), \delta(t_N; \theta)) = \nabla_\theta x(t_N; \theta)^\top \gamma
\]
for any vector $\gamma$. Then, building on the discussion in Section 2.1, we see that solving the adjoint system (3.2) backwardly with the final states
\[
\xi(t_N) = \nabla_x \tilde{C}(x(t_N; \theta), \delta(t_N; \theta)) = (H_x C(x(t_N; \theta))) \delta(t_N; \theta)
\]
and
\[
\lambda(t_N) = \nabla_\theta \tilde{C}(x(t_N; \theta), \delta(t_N; \theta)) = \nabla_x C(x(t_N; \theta))
\]
leads to the Hessian-vector multiplication at $t = 0$, i.e.
\[
\xi(0) = \nabla_\theta \tilde{C}(x(t_N; \theta), \delta(t_N; \theta)) = (H_\theta C(x(t_N; \theta))) \gamma
\]
as well as the gradient
\[
\lambda(0) = \nabla_\theta \tilde{C}(x(t_N; \theta), \delta(t_N; \theta)) = \nabla_\theta C(x(t_N; \theta)).
\]

We note that the discussion of this subsection makes it possible to discuss the second-order adjoint system within the framework of (first-order) adjoint systems.

3.2 Exact Hessian-vector multiplication

From the discussion in Sections 2.2 and 3.1, we readily see that the exact Hessian-vector multiplication $(H_\theta C(x(t_N; \theta))) \gamma$ is obtained by solving the coupled adjoint system (3.2) with a particular choice of Runge–Kutta method.

Suppose that the pair of $x$- and $\delta$-systems (3.1) is discretized by a Runge–Kutta method:

$$x_{n+1} = x_n + h \sum_{i=1}^s b_i k_{n,i},$$

$$k_{n,i} = f(X_{n,i}), \quad i = 1, \ldots, s,$$

$$X_{n,i} = x_n + h \sum_{j=1}^s a_{ij} k_{n,j}, \quad i = 1, \ldots, s,$$
and
\[ \delta_{n+1} = \delta_n + h \sum_{i=1}^{s} b_i \tilde{k}_{n,i}, \]
\[ \tilde{k}_{n,i} = \nabla_x f(X_{n,i}) D_{n,i}, \quad i = 1, \ldots, s, \]
\[ D_{n,i} = \delta_n + h \sum_{j=1}^{s} a_{ij} \tilde{k}_{n,j}, \quad i = 1, \ldots, s. \]

We discretize the adjoint system (3.2), i.e. the pair of \( \xi \)- and \( \lambda \)-systems, by another Runge–Kutta method:
\[ \lambda_{n+1} = \lambda_n + h \sum_{i=1}^{s} B_{i} l_{n,i}, \]
\[ l_{n,i} = -\nabla_x f(X_{n,i})^\top \Lambda_{n,i}, \quad i = 1, \ldots, s, \]
\[ \Lambda_{n,i} = \lambda_n + h \sum_{j=1}^{s} A_{ij} l_{n,j}, \quad i = 1, \ldots, s, \]
and
\[ \xi_{n+1} = \xi_n + h \sum_{i=1}^{s} B_{i} \tilde{l}_{n,i}, \]
\[ \tilde{l}_{n,i} = -\nabla_x f(X_{n,i})^\top \Xi_{n,i} - (\nabla_x f(X_{n,i}) D_{n,i})^\top \Lambda_{n,i}, \quad i = 1, \ldots, s, \]
\[ \Xi_{n,i} = \xi_n + h \sum_{j=1}^{s} A_{ij} \tilde{l}_{n,j}, \quad i = 1, \ldots, s. \]

Then, the following theorem is immediate.

**Theorem 3.1** Assume that the coefficients \( A_{ij} \) and \( B_{i} \) of the Runge–Kutta method for the (coupled) adjoint system (3.2) satisfy the relation
\[ b_{i} = B_{i}, \quad i = 1, \ldots, s, \]
\[ b_{i} A_{ij} + B_{j} a_{ji} = b_{j} B_{j}, \quad i, j = 1, \ldots, s. \]

Then, solving the adjoint system with \( \xi_N = (H_th C(x_N(\theta))) \gamma \) and \( \lambda_N = \nabla_x C(x_N(\theta)) \) gives the exact Hessian-vector multiplication at \( n = 0 \), i.e. \( \xi_0 = (H_0 h C(x_N(\theta))) \gamma \) as well as the exact gradient \( \lambda_0 = \nabla_\theta C(x_N(\theta)) \).

### 3.3 Numerical verification

We verify the discussion of Section 3.2 by a numerical experiment for the simple pendulum problem

\[ \frac{d}{dt} \begin{bmatrix} q \\ p \end{bmatrix} = \begin{bmatrix} p \\ -\sin(q) \end{bmatrix}, \quad \begin{bmatrix} q(0) \\ p(0) \end{bmatrix} = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}, \quad (3.3) \]
which is employed as a toy problem. We discretize this system (3.3) by the explicit Euler method. The function $C$ is defined by $C(x) = C(q,p) = q^2 + qp + p^2 + p^4$. The following numerical experiments are carried out by using Julia language.

The step size is set to $h = 0.01$. As a reference, we obtain the exact Hessian $H_{\theta}C(x_5(\theta))\big|_{\theta=[1,1]}$ at $N=5$ with the help of symbolic computation. We use SymPy package in Julia. Note that symbolic computation is possible only when $N$ is relatively small. The result is

$$H_{\theta}C(x_5(\theta))\big|_{\theta=[1,1]} = \begin{bmatrix} 2.232746371638453 & 0.7631322035490988 \\ 0.7631322035490988 & 13.091167393760282 \end{bmatrix}.$$  (3.4)

We compute $\xi_0$ using the proposed approach. We employ two vectors $[1,0]^T$ and $[0,1]^T$ as $\gamma$ to obtain the exact Hessian, and the result is

$$\begin{bmatrix} 2.232746371638453 & 0.7631322035490989 \\ 0.7631322035490999 & 13.091167393760278 \end{bmatrix},$$

which coincides with (3.4) to 14 digits. For comparison, we discretize the adjoint system (3.2), i.e. the pair of the (first-order) adjoint system and second-order adjoint system, by the implicit Euler method, and obtain the approximated Hessian

$$\begin{bmatrix} 2.2346793074348708 & 0.7714498126733377 \\ 0.7631693902666702 & 13.091333764244673 \end{bmatrix},$$

which differs from (3.4) substantially. We also note that this matrix is no longer symmetric.

### 4 Conclusion

In this paper, we have shown a concise derivation of the second-order adjoint system, and a procedure for computing a matrix-vector multiplication exactly, where the matrix is the Hessian of a function of the numerical solution of an initial value problem with respect to the initial data. The fact that the second-order adjoint system can be reformulated to a part of a large adjoint system is the key point to obtain the exact Hessian-vector multiplication based on the Sanz-Serna scheme.

The proposed method can be used either to obtain the exact Hessian or to solve a linear system having the Hessian as the coefficient matrix based on a Krylov subspace method. Particularly in the latter case, the proposed method can contribute a rapid convergence since the accuracy of Hessian-vector multiplication affects the speed of convergence directly.

It would be of interest to apply the method to more practical problems, and we plan to test the method to quantify the uncertainty for the estimation of such problems. We note that in many applications an ODE system often arises from discretizing a time-dependent partial differential equation (PDE) in space. However, discretizing PDEs in space before taking the adjoint may lead to a very strong nonphysical behaviour [8] (this issue has been partially addressed in [10]). Since the proposed method does not care about the spatial discretization, we have to take the spatial
discretization into account when testing the proposed method to practical problems. Considering with such spatial discretization may provide an optimal combination of time and spatial discretizations for given problems.

Acknowledgements This work was triggered by discussions in the research projects of JST CREST Grant Number JPMJCR1761, JST ACT-I Grant Number JPMJPR18US, JSPS Grants-in-Aid for Scientific Research (B) Grant Number 17H01703, and JSPS Grants-in-Aid for Early-Career Scientists Grant Numbers 16K17550, 19K14671 and 19K20220.

References

1. Abia, L., Sanz-Serna, J.M.: Partitioned Runge–Kutta methods for separable Hamiltonian problems. Math. Comp. 60(202), 617–634 (1993). DOI 10.2307/2153105
2. Dunet, F.X.L., Talagrand, O.: Variational algorithms for analysis and assimilation of meteorological observations: theoretical aspects. Tellus A 38A(2), 97–110 (1986). DOI 10.1111/j.1600-0870.1986.th00459.x
3. Fichtner, A., Bunge, H.P., Igel, H.: The adjoint method in seismology: I. theory. Physics of the Earth and Planetary Interiors 157(1), 86–104 (2006). DOI https://doi.org/10.1016/j.pepi.2006.03.016
4. Giles Michael B.and Pierce, N.A.: An introduction to the adjoint approach to design. Flow, Turbulence and Combustion 65(3), 393–415 (2000). DOI 10.1023/A:1011430410075
5. Hairer, E., Lubich, C., Wanner, G.: Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential equations, second edn. Springer-Verlag, Berlin (2006)
6. Ito, S., Nagao, H., Yamanaka, A., Tsukada, Y., Koyama, T., Kano, M., Inoue, J.: Data assimilation for massive autonomous systems based on a second-order adjoint method. Phys. Rev. E 94(4), 043307 (2016). DOI 10.1103/PhysRevE.94.043307
7. Sanz-Serna, J.M.: Symplectic Runge–Kutta schemes for adjoint equations, automatic differentiation, optimal control, and more. SIAM Rev. 58(1), 3–33 (2016). DOI 10.1137/15M1002769
8. Sirkes, Z., Tziperman, E.: Finite difference of adjoint or adjoint of finite difference? Mon. Weather Rev. 125(12), 3373–3378 (1997). DOI 10.1175/1520-0493(1997)125⟨3373:fdoaao⟩2.0.co;2
9. Sun, G.: Symplectic partitioned Runge–Kutta methods. J. Comput. Math. 11(4), 365–372 (1993)
10. Tanaka, T., Matsuo, T., Ito, S., Nagao, H.: Making adjacent discretizations consistent in partial differential equations. In preparation
11. Thacker, W.C.: The role of the hessian matrix in fitting models to measurements. J. Geophys. Res. Oceans 94(C5), 6177–6196 (1989). DOI 10.1029/JC094iC05p06177
12. Wang, Z., Droegemeier, K., White, L.: The adjoint Newton algorithm for large-scale unconstrained optimization in meteorology applications. Comput. Optim. and Appl. 10(3), 283–320 (1998). DOI 10.1023/A:1018321307393
13. Wang, Z., Navon, I.M., Dimet, F.X.L., Zou, X.: The second order adjoint analysis: Theory and applications. Meteor. Atmos. Phys. 50(1-3), 3–20 (1992). DOI 10.1007/bf01025501