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Author for correspondence:
Derek Harland
e-mail: D.G.Harland@leeds.ac.uk

Approximating the parallel transport of an induced connection

Derek Harland

School of Mathematics, University of Leeds, Leeds LS2 9JT, UK

DH, 0000-0002-4110-9673

Efficient numerical methods to approximate the parallel transport operators of the induced connection on a sub-bundle of a vector bundle are presented. These methods are simpler than naive applications of a Runge–Kutta algorithm and have accuracy up to order 4. They have the desirable property of being insensitive to choices of trivialization of the sub-bundle. The methods were developed to solve a problem of computing skyrmions using the Atiyah–Manton–Sutcliffe and Atiyah–Drinfeld–Hitchin–Manin constructions, but are applicable to a broader range of problems in computational geometry.

1. Introduction

Given a hermitian vector bundle equipped with a unitary connection ∇, any sub-bundle E comes equipped with a natural connection ∇^E. The covariant derivative $\nabla^E s$ of any section s of E is defined to be the orthogonal projection of ∇s onto E. Induced connections feature prominently in submanifold geometry, where the tangent and normal bundles of a submanifold inherit natural connections from the Levi-Civita connection of the ambient manifold, and in quantum mechanics, where they are known as Berry connections. They also play a central role in the Atiyah–Drinfeld–Hitchin–Manin (ADHM) construction of instantons, which constructs solutions of the anti-self-dual Yang–Mills equation using induced connections (for reviews, see [1–4]).

A fundamental property of any connection is the collection of its parallel transport operators. These are linear maps between fibres $E_p \to E_q$ that depend on

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a choice of curve γ from p to q. They determine the holonomy group of the connection, and in discrete geometry, they are used to form a discrete representation of the connection [5]. Parallel transport operators of induced connections arise naturally in quantum mechanics, e.g. where they are known as Berry phases. The main result of this note is a collection of high-order numerical methods to approximate the parallel transport operators of an induced connection.

The results that we presented here are motivated by the ongoing work to approximate skyrmions using the Atiyah–Manton–Sutcliffe construction [6–18]. This construction approximates soliton solutions of a nonlinear field theory, the Skyrme model, using parallel transport operators of Yang–Mills instantons. The simplest and most effective way of constructing instantons is the ADHM method, which uses induced connections. To obtain a skyrmion from an instanton entails computing hundreds of parallel transports. Moreover, to compute quantities relevant to applications in nuclear physics, one may need to compute skyrmions from hundreds of different instantons. So an efficient and accurate method to compute parallel transport of an induced connection is highly desirable in this context.

Computing parallel transport amounts to solving an initial value problem

$$\Omega'(x,0) = -A(x)\Omega(x,0) \quad \text{and} \quad \Omega(0,0) = \mathrm{Id}, \tag{1.1}$$

where $A = V^\dagger \nabla_{\gamma'} V$ is the connection matrix with respect to a chosen orthonormal frame $V(x)$. The most obvious method to compute Ω (used, e.g. in [14]) is to first find an orthonormal frame $V(x_i)$ at a finite set of points $x_1, \ldots, x_n$ (using a Gram–Schmidt algorithm), then approximate A using finite differences and finally approximate the solution Ω using a Runge–Kutta method.

There are two problems with this naive method. The first is that it is not gauge-covariant. The matrix $\Omega(x,0)$ represents a linear map between the fibres of E at 0 and x, so depends on the choice of bases $V(0)$ and $V(x)$, but does not depend on the choice of bases $V(w)$ at intermediate points $0 < w < x$. However, any approximate solution obtained using the naive method described earlier would depend on $V(w)$ at intermediate points w. In particular, if $V(w)$ happens to depend on w in a discontinuous way, then the accuracy of methods such as Runge–Kutta (which assume analyticity of all functions involved) is questionable. A second criticism of the naive method is that it is inefficient. It entails computing derivatives (to obtain A) and then partially undoing this by computing integrals (to solve the parallel transport equation).

The methods that we present below compute parallel transport directly from $V(x)$, and so avoid this inefficiency. Our methods are derived using an algebraic approach that raises some intriguing questions and may be of independent mathematical interest.

Given the ubiquity of induced connections, it seems likely that our results will prove useful in other contexts. We sketch one possible further application to the geometry of curves at the end of §4. An outline of this article is as follows: in §2, we establish our notation and derive some simple approximations to parallel transport. In §3, we introduce an operator formalism and use this to derive more sophisticated approximations to parallel transport. In §4, we illustrate our method in a simple example and describe some applications. Section 5 discusses some interesting theoretical questions about our method.

2. Simple approximations to parallel transport

(a) Statement of the problem

Throughout this article, we will take our ambient vector bundle to be the trivial bundle $\mathbb{C}^n \times \mathbb{R}$ over the manifold $\mathbb{R}$, equipped with the standard hermitian metric and the trivial connection. No generality is lost here, because parallel transport is always defined along a one-dimensional submanifold of the ambient manifold, and all vector bundles and connections over $\mathbb{R}$ are trivial.

We will let E be a rank m sub-bundle with orthonormal frame $v^1, \ldots, v^m$. This means that, for each $x \in \mathbb{R}$, the fibre E_x is the span of vectors $v^1(x), \ldots, v^m(x)$ satisfying $v^i(x)^\dagger v^j(x) = \delta_{ij}$. Let V be

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the $n \times m$ matrix-valued function whose columns are $v^1, \dots v^m$; note that $V^\dagger V = \mathrm{Id}_m$. A section of E can be written in the following form:

$$z(x) = V(x)y(x), \quad y : \mathbb{R} \to \mathbb{C}^m. \tag{2.1}$$

A section z is parallel if $z' \in E^\perp$. This is equivalent to $V^\dagger z' = 0$, which is in turn equivalent to

$$y'(x) + A(x)y(x) = 0, \quad A(x) := V(x)^\dagger V'(x). \tag{2.2}$$

Equation (2.2) is known as the parallel transport equation, and $A = V^\dagger V'$ is the matrix of the induced connection.

The solution of the parallel transport equation with initial condition $y(x_0) = y_0$ can be written as follows:

$$y(x) = \Omega(x, x_0)y_0, \tag{2.3}$$

where Ω is a $U(m)$-valued function, called the parallel transport operator. The parallel transport operator is the unique solution to

$$\frac{\mathrm{d}}{\mathrm{d}x}\Omega(x, x_0) + A(x)\Omega(x, x_0) = 0, \quad \Omega(x_0, x_0) = \mathrm{Id}_m. \tag{2.4}$$

Gauge transformations $g : \mathbb{R} \to U(m)$ correspond to an x-dependent change of basis. They act as

$$V(x) \mapsto V(x)g(x) \quad \text{and} \quad y(x) \mapsto g(x)^\dagger y(x). \tag{2.5}$$

The induced action on the parallel transport operator is

$$\Omega(x, x_0) \mapsto g(x)^\dagger \Omega(x, x_0)g(x_0). \tag{2.6}$$

The goal of this article is to find approximations $\Omega^k(x + h, x)$ to $\Omega(x + h, x)$, such that

$$\Omega(x + h, x) = \Omega^k(x + h, x) + O(h^{k+1}). \tag{2.7}$$

Our approximations will be written as rational functions of $V(x_i)$ for a finite set of points $x_0 < x_1 < x_2 < \cdots$. We will require that, under gauge transformations, $V(x_i) \mapsto V(x_i)g(x_i)$, Ω^k transforms in the same way as Ω:

$$\Omega^k(x + h, x) \mapsto g(x + h)^\dagger \Omega^k(x + h, x)g(x). \tag{2.8}$$

(b) Order 2 approximation

A simple solution to this problem (used earlier in [9]) is

$$\Omega^1(x + h, x) = V(x + h)^\dagger V(x). \tag{2.9}$$

Notice that under gauge transformations, $V(x + h)^\dagger V(x) \mapsto g(x + h)^\dagger V(x + h)^\dagger V(x)g(x)$, so Ω^1 transforms in the desired way.

To see that the approximation is order 1, we use Taylor expansions. The parallel transport equation (2.2) implies that

$$y' = -V^\dagger V' y, \tag{2.10}$$

$$y'' = -(V')^\dagger V' y - V^\dagger V'' y - V^\dagger V' y' \tag{2.11}$$

$$= (-(V')^\dagger V' - V^\dagger V'' + (V^\dagger V')^2)y. \tag{2.12}$$

So

$$\Omega(x + h, x)y(x) = y(x + h) \tag{2.13}$$

$$= y(x) + hy'(x) + \frac{h^2}{2}y''(x) + O(h^3) \tag{2.14}$$

$$= \left[1 - hV^\dagger V' + \frac{h^2}{2}(-(V')^\dagger V' - V^\dagger V'' + (V^\dagger V')^2)\right] y + O(h^3), \tag{2.15}$$

where in the last line, y, V, V', V'' are understood to be evaluated at x. Conversely,

$$V(x+h)^\dagger V(x) = \left[V(x) + hV'(x) + \frac{h^2}{2}V''(x) + O(h^3)\right]^\dagger V(x) \tag{2.16}$$

$$= V^\dagger V + h(V')^\dagger V + \frac{h^2}{2}(V'')^\dagger V + O(h^3) \tag{2.17}$$

$$= 1 - hV^\dagger V' - h^2\left((V')^\dagger V' + \frac{1}{2}V^\dagger V''\right) + O(h^3), \tag{2.18}$$

where in the last line, we used $V^\dagger V = \mathrm{Id}_m$, $(V')^\dagger V + V^\dagger V' = 0$ and $(V'')^\dagger V + 2(V')^\dagger V' + V^\dagger V'' = 0$. Comparing the two calculations, we see that $\Omega(x+h, x) = V^\dagger(x+h)V(x) + O(h^2)$.

To improve this method, we seek a second-order approximation in the following form:

$$\Omega^2(x+h, x) = aV(x+h)^\dagger V(x) + b[V(x)^\dagger V(x+h)]^{-1}, \tag{2.19}$$

where $a, b \in \mathbb{R}$ are to be determined. Note that the choice of operators on the right ensures that Ω^2 transforms in the desired way under gauge transformations. To compare this with Ω, we need the Taylor expansion of the second operator:

$$[V(x)^\dagger V(x+h)]^{-1} = \left[V^\dagger V + hV^\dagger V' + \frac{h^2}{2}V^\dagger V'' + O(h^3)\right]^{-1} \tag{2.20}$$

$$= 1 - hV^\dagger V' + h^2\left((V^\dagger V')^2 - \frac{1}{2}V^\dagger V''\right) + O(h^3). \tag{2.21}$$

So our approximation is

$$aV(x+h)^\dagger V(x) + b[V(x)^\dagger V(x+h)]^{-1}$$

$$= (a+b)(1 - hV^\dagger V') + h^2\left(-\frac{a+b}{2}V^\dagger V'' - a(V')^\dagger V' + b(V^\dagger V')^2\right) + O(h^3). \tag{2.22}$$

This agrees with the expansion (2.15) of Ω precisely when $a = b = \frac{1}{2}$. So our order two method is

$$\Omega^2(x+h, x) = \frac{1}{2}(V(x+h)^\dagger V(x) + [V(x)^\dagger V(x+h)]^{-1}). \tag{2.23}$$

3. Higher order approximations

(a) An operator expression for Ω

The method used earlier to derive a second-order approximation can in principle be used to derive higher order approximations. However, in practice, the algebra quickly becomes cumbersome. In this section, we derive an operator expression for Ω that allows for much simpler derivations of approximations Ω^k.

Let $\Gamma(E)$ be the space of sections of E, or more precisely, the set of functions $z : \mathbb{R} \to \mathbb{C}^n$ such that $VV^\dagger z = z$. Consider the operator $\omega(h) : \Gamma(E) \to \Gamma(E)$ defined by

$$(\omega(h)z)(x) = V(x)\Omega(x, x-h)V^\dagger(x-h)z(x-h). \tag{3.1}$$

The matrices $\Omega(x+h, x)$ determine, and are determined by, the operators $\omega(h)$. The advantage of introducing the operators $\omega(h)$ is that they can be expressed in the following simple way:

$$\omega(h)z = V\exp(-h(D + A))V^\dagger z. \tag{3.2}$$

In this expression, D denotes the operator $\mathrm{d}/\mathrm{d}x$, and $V, V^\dagger, A$ act on vector-valued functions by matrix multiplication.

To show that the right-hand sides of (3.2) and (3.1) are equal, we first consider the case where $h = 0$. In this situation, both (3.2) and (3.1) correspond to multiplying $z(x)$ with the identity matrix, so they agree.

To show that they agree for all values of h, we differentiate both:

$$\left(\frac{\partial}{\partial x}+\frac{\partial}{\partial h}\right)V(x)\Omega(x,x-h)V^\dagger(x-h)z(x-h) \tag{3.3}$$

$$=(V'(x)-V(x)A(x))\Omega(x,x-h)V^\dagger(x-h)z(x-h) \tag{3.4}$$

$$=(V'V^\dagger-VAV^\dagger)V(x)\Omega(x,x-h)V^\dagger(x-h)z(x-h) \tag{3.5}$$

and

$$\left(\frac{\partial}{\partial x}+\frac{\partial}{\partial h}\right)(V\exp(-h(D+A))V^\dagger z) \tag{3.6}$$

$$=D(V\exp(-h(D+A))V^\dagger z)-V(D+A)\exp(-h(D+A))V^\dagger z \tag{3.7}$$

$$=([D,V]-VA)\exp(-h(D+A))V^\dagger z \tag{3.8}$$

$$=(V'V^\dagger-VAV^\dagger)V\exp(-h(D+A))V^\dagger z. \tag{3.9}$$

In the first of these calculations, we used the parallel transport equation (2.4), and in both calculations, we inserted a factor of $V^\dagger V=\mathrm{Id}_m$. We find that the operators $\omega(h)$ defined by both (3.1) and (3.2) satisfy

$$\frac{\partial}{\partial h}\omega(h)=(-D-VAV^\dagger+V'V^\dagger)\omega(h). \tag{3.10}$$

Since the two operators satisfy the same differential equation and agree when $h=0$, they agree for all values of h.

It will prove convenient to rewrite (3.2) as follows. Since $V^\dagger V=\mathrm{Id}_m$ and $A=V^\dagger[D,V]$, we have that $D+A=V^\dagger DV$. Therefore,

$$\omega(h)=V\exp(-hV^\dagger DV)V^\dagger \tag{3.11}$$

$$=1-hPD+\frac{h^2}{2}PDPD-\frac{h^3}{6}PDPDPD+\frac{h^4}{24}PDPDPDPD+O(h^5), \tag{3.12}$$

in which we have introduced the projection operator $P=VV^\dagger$ onto $\Gamma(E)$. Note that $Pz=z$ for any $z\in\Gamma(E)$; we have used this fact (and the fact that $\omega(h)$ acts on $\Gamma(E)$) to eliminate operators P from the right of all products in (3.12). We now seek operators $\omega^k(h)$ that approximate $\omega(h)$ and from these deduce approximations to $\Omega(x+h,x)$.

(b) Order 2

We begin by rederiving the second-order expression obtained earlier. We seek an approximation $\omega^2(h)$ to $\omega(h)$ using the operators $\pi_1,\pi_2:\Gamma(E)\to\Gamma(E)$ defined by

$$(\pi_1(h)z)(x)=V(x)V^\dagger(x)z(x-h) \tag{3.13}$$

and

$$\pi_2(h)=\pi_1(-h)^{-1}. \tag{3.14}$$

We obtain Taylor expansions as follows:

$$\pi_1(h)=VV^\dagger\exp(-hD) \tag{3.15}$$

$$=1-hPD+\frac{h^2}{2}PD^2+O(h^3) \tag{3.16}$$

and

$$\pi_2(h)=\left(1+hPD+\frac{h^2}{2}PD^2\right)^{-1}+O(h^3) \tag{3.17}$$

$$=1-hPD-\frac{h^2}{2}PD^2+h^2PDPD+O(h^3). \tag{3.18}$$

Once again, we have used the fact that $P = VV^\dagger$ acts as the identity on $\Gamma(E)$.

If we compare equations (3.16) and (3.18) with the expansion (3.12) of $\omega(h)$, it is clear that

$$\omega^2(h) = \frac{1}{2}(\pi_1(h) + \pi_2(h)) \tag{3.19}$$

is a second-order approximation to $\omega(h)$.

To compare equation (3.19) with our earlier approximation (2.23) to Ω, we rewrite $\pi_1(h)$ and $\pi_2(h)$ as follows:

$$(\pi_1(h)z)(x) = V(x)[V^\dagger(x)V(x-h)]V^\dagger(x-h)z(x-h) \tag{3.20}$$

and

$$(\pi_2(h)z)(x) = V(x)[V^\dagger(x-h)V(x)]^{-1}V^\dagger(x-h)z(x-h). \tag{3.21}$$

The first of these is obtained from (3.13) using the fact that $VV^\dagger z = z$ for $z \in \Gamma(E)$, and it can be checked that the second satisfies $\pi_2(h)\pi_1(-h) = \pi_1(-h)\pi_2(h) = 1$, as required by (3.14). From these, it follows that ω^2 and Ω^2 given in (3.19) and (2.23) satisfy

$$(\omega^2(h)z)(x) = V(x)\Omega^2(x, x-h)V^\dagger(x-h)z(x-h), \tag{3.22}$$

and by comparing with (3.1), we see that ω^2 reproduces our earlier approximation Ω^2.

(c) Order 3

To obtain an order 3 approximation, we consider an ansatz

$$\omega^3(h) = a_1\omega^2\left(\frac{h}{2}\right)\omega^2\left(\frac{h}{2}\right) + a_2\,\omega^2(h). \tag{3.23}$$

To compare this with (3.12), we need an expansion for ω^2. This is obtained in a similar way to the expansions (3.16) and (3.18):

$$\begin{aligned}\omega^2(h) = 1 - hPD + \frac{h^2}{2}PDPD \\ + h^3\left(-\frac{1}{6}PD^3 + \frac{1}{4}PD^2PD + \frac{1}{4}PDPD^2 - \frac{1}{2}PDPDPD\right) \\ + h^4\left(\frac{1}{12}PD^3PD + \frac{1}{8}PD^2PD^2 + \frac{1}{12}PDPD^3 - \frac{1}{4}PD^2PDP\,D\right. \\ \left. -\frac{1}{4}PDPD^2PD - \frac{1}{4}PDPDPD^2 + \frac{1}{2}PDPDPDPD\right) + O(h^5).\end{aligned} \tag{3.24}$$

From this, it follows that

$$\begin{aligned}\omega^2(\tfrac{h}{2})\omega^2(\tfrac{h}{2}) = 1 - hPD + \frac{h^2}{2}PDPD + h^3\left(-\frac{1}{24}PD^3\right. \\ \left. +\frac{1}{16}PDPD^2 + \frac{1}{16}PD^2PD - \frac{1}{4}PDPDPD\right) + O(h^4).\end{aligned} \tag{3.25}$$

By comparing these two expansions with (3.12), we see that ω^3 given in (3.23) is an order 3 approximation to ω if and only if

$$\begin{pmatrix} 1 & 1 \\ -1 & -1 \\ \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{24} & -\frac{1}{6} \\ \frac{1}{16} & \frac{1}{4} \\ \frac{1}{16} & \frac{1}{4} \\ -\frac{1}{4} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ \frac{1}{2} \\ 0 \\ 0 \\ 0 \\ -\frac{1}{6} \end{pmatrix}. \tag{3.26}$$

The unique solution is $a_1 = \frac{4}{3}$ and $a_2 = -\frac{1}{3}$. The corresponding order 3 approximation to Ω is

$$\Omega^3(x+h,x) = \frac{4}{3}\Omega^2\left(x+h, x+\frac{h}{2}\right)\Omega^2\left(x+\frac{h}{2}, x\right) - \frac{1}{3}\Omega^2(x+h,x). \tag{3.27}$$

(d) Order 4

To obtain an order 4 approximation, we consider operators of the following form:

$$\omega^4(h) = a_1\omega^2\left(\frac{h}{3}\right)\omega^2\left(\frac{h}{3}\right)\omega^2\left(\frac{h}{3}\right) + a_2\omega^2\left(\frac{h}{3}\right)\omega^2\left(\frac{2h}{3}\right) + a_3\omega^2\left(\frac{2h}{3}\right)\omega^2\left(\frac{h}{3}\right) + a_4\omega^2(h). \tag{3.28}$$

The expansion of the final operator appearing on the right is given in (3.24), and the expansions of the remaining three operators can all be derived from (3.24):

$$\begin{aligned} &\omega^2\left(\frac{h}{3}\right)\omega^2\left(\frac{h}{3}\right)\omega^2\left(\frac{h}{3}\right) \\ &\quad = 1 - hPD + \frac{h^2}{2}PDPD \\ &\qquad + h^3\left(-\frac{1}{54}PD^3 + \frac{1}{36}PD^2PD + \frac{1}{36}PDPD^2 - \frac{11}{54}PDPDPD\right) \\ &\qquad + h^4\left(\frac{1}{108}PD^3PD + \frac{1}{216}PD^2PD^2 + \frac{1}{108}PDPD^3 - \frac{1}{54}PD^2PDPD\right. \\ &\qquad \left. - \frac{1}{36}PDPD^2PD - \frac{1}{54}PDPDPD^2 + \frac{1}{12}PDPDPDPD\right) + O(h^5), \end{aligned} \tag{3.29}$$

$$\begin{aligned} &\omega^2\left(\frac{h}{3}\right)\omega^2\left(\frac{2h}{3}\right) \\ &\quad = 1 - hPD + \frac{h^2}{2}PDPD \\ &\qquad + h^3\left(-\frac{1}{18}PD^3 + \frac{1}{12}PD^2PD + \frac{1}{12}PDPD^2 - \frac{5}{18}PDPDPD\right) \\ &\qquad + h^4\left(\frac{7}{324}PD^3PD + \frac{17}{648}PD^2PD^2 + \frac{11}{324}PDPD^3 - \frac{19}{324}PD^2PDPD\right. \\ &\qquad \left. - \frac{1}{12}PDPD^2PD - \frac{25}{324}PDPDPD^2 + \frac{29}{162}PDPDPDPD\right) + O(h^5) \end{aligned} \tag{3.30}$$

and

$$\begin{aligned}
&\omega^2\left(\frac{2h}{3}\right)\omega^2\left(\frac{h}{3}\right)\\
&=1-hPD+\frac{h^2}{2}PDPD\\
&\quad+h^3\left(-\frac{1}{18}PD^3+\frac{1}{12}PD^2PD+\frac{1}{12}PDPD^2-\frac{5}{18}PDPDPD\right)\\
&\quad+h^4\left(\frac{11}{324}PD^3PD+\frac{17}{648}PD^2PD^2+\frac{7}{324}PDPD^3-\frac{25}{324}PD^2PDPD\right.\\
&\quad\left.-\frac{1}{12}PDPD^2PD-\frac{19}{324}PDPDPD^2+\frac{29}{162}PDPDPDPD\right)+O(h^5).
\end{aligned}\tag{3.31}$$

It follows that ω^4 given in equation (3.28) is an order 4 approximation to ω given in (3.12) if and only if a_1, a_2, a_3 and a_4 satisfy the linear equation,

$$\begin{pmatrix}
1 & 1 & 1 & 1\\
-1 & -1 & -1 & -1\\
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2}\\
-\frac{1}{54} & -\frac{1}{18} & -\frac{1}{18} & -\frac{1}{6}\\
\frac{1}{36} & \frac{1}{12} & \frac{1}{12} & \frac{1}{4}\\
\frac{1}{36} & \frac{1}{12} & \frac{1}{12} & \frac{1}{4}\\
-\frac{11}{54} & -\frac{5}{18} & -\frac{5}{18} & -\frac{1}{2}\\
\frac{1}{108} & \frac{7}{324} & \frac{11}{324} & \frac{1}{12}\\
\frac{1}{216} & \frac{17}{648} & \frac{17}{648} & \frac{1}{8}\\
\frac{1}{108} & \frac{11}{324} & \frac{7}{324} & \frac{1}{12}\\
-\frac{1}{54} & -\frac{19}{324} & -\frac{25}{324} & -\frac{1}{4}\\
-\frac{1}{36} & -\frac{1}{12} & -\frac{1}{12} & -\frac{1}{4}\\
-\frac{1}{54} & -\frac{25}{324} & -\frac{19}{324} & -\frac{1}{4}\\
\frac{1}{12} & \frac{29}{162} & \frac{29}{162} & \frac{1}{2}
\end{pmatrix}\begin{pmatrix}a_1\\a_2\\a_3\\a_4\end{pmatrix}=\begin{pmatrix}
1\\-1\\\frac{1}{2}\\0\\0\\0\\-\frac{1}{6}\\0\\0\\0\\0\\0\\0\\\frac{1}{24}
\end{pmatrix}.\tag{3.32}$$

The unique solution is given by $(a_1, a_2, a_3, a_4) = \frac{1}{44}(90, -27, -27, 8)$. So our order 4 approximation to Ω is

$$\begin{aligned}
\Omega^4(x+h,x)=\frac{1}{44}&\left(90\Omega^2\left(x+h,x+\frac{2h}{3}\right)\Omega^2\left(x+\frac{2h}{3},x+\frac{h}{3}\right)\Omega^2\left(x+\frac{h}{3},x\right)\right.\\
&-27\Omega^2\left(x+h,x+\frac{2h}{3}\right)\Omega^2\left(x+\frac{2h}{3},x\right)\\
&\left.-27\Omega^2\left(x+h,x+\frac{h}{3}\right)\Omega^2\left(x+\frac{h}{3},x\right)+8\Omega^2(x+h,x)\right).
\end{aligned}\tag{3.33}$$

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(e) Improved methods

The connection matrix $A = V^\dagger V'$ that appears in the parallel transport equation (2.2) is anti-hermitian. It follows that $\Omega(x+h,x)$ is a unitary $m \times m$ matrix, and hence that

$$|\det(\Omega(x+h,x))| = 1. \tag{3.34}$$

Therefore,

$$\widehat{\Omega}^k(x+h,x) := |\det(\Omega^k(x+h,x))|^{-(1/m)}\Omega^k(x+h,x) \tag{3.35}$$

satisfies $|\det(\widehat{\Omega}^k(x+h,x))| = 1$ and hence is a better approximation to parallel transport that Ω^k. In fact, in certain situations, $\widehat{\Omega}^k(x+h,x) - \Omega(x+h,x) = O(h^{k+2})$, so this improved approximation is an order of magnitude better than Ω^k. We review these situations below.

The first case to consider is where our sub-bundle E has rank 1. In this case, Ω^k is a 1×1 matrix, and so

$$\det(\Omega^k(x+h,x)) = \Omega^k(x+h,x). \tag{3.36}$$

Since $\Omega(x+h,x)$ is unitary and $\Omega(x+h,x)^{-1} = \Omega(x,x+h)$, we have that

$$\Omega(x+h,x)^\dagger = \Omega(x,x+h). \tag{3.37}$$

We will assume similarly that

$$\Omega^k(x+h,x)^\dagger = \Omega^k(x,x+h). \tag{3.38}$$

This assumption is satisfied by all of the approximations Ω^1, Ω^2, Ω^3 and Ω^4 obtained earlier. Now we introduce $\epsilon^k(x)$ such that

$$\Omega^k(x+h,x) = \Omega(x+h,x) + h^{k+1}\epsilon^k(x) + O(h^{k+2}). \tag{3.39}$$

It follows that

$$\Omega^k(x,x+h) = \Omega(x,x+h) + (-h)^{k+1}\epsilon^k(x+h) + O(h^{k+2}) \tag{3.40}$$

$$= \Omega(x,x+h) + (-h)^{k+1}\epsilon^k(x) + O(h^{k+2}), \tag{3.41}$$

because $\epsilon^k(x+h) = \epsilon^k(x) + O(h)$. Therefore,

$$|\det(\Omega^k(x+h,x))|^2 = \Omega^k(x+h,x)\Omega^k(x+h,x)^\dagger \quad \text{by (3.36)} \tag{3.42}$$

$$= \Omega^k(x+h,x)\Omega^k(x,x+h) \quad \text{by (3.38)} \tag{3.43}$$

$$= (\Omega(x+h,x) + h^{k+1}\epsilon^k(x)) \times (\Omega(x,x+h) + (-h)^{k+1}\epsilon^k(x)) + O(h^{k+2}) \tag{3.44}$$

$$= 1 + \left[1 + (-1)^{k+1}\right]h^{k+1}\epsilon^k + O(h^{k+2}). \tag{3.45}$$

Here, in the final line, we used that $\Omega(x+h,x)\Omega(x,x+h) = 1$ and that $\Omega(x+h,x) = 1 + O(h)$.

Thus, in the case that k is odd, we obtain

$$\widehat{\Omega}^k(x+h,x) = \Omega^k(x+h,x)(1 + 2h^{k+1}\epsilon^k)^{-(1/2)} + O(h^{k+2}) \tag{3.46}$$

$$= (\Omega(x+h,x) + h^{k+1}\epsilon^k)(1 - h^{k+1}\epsilon^k) + O(h^{k+2}) \tag{3.47}$$

$$= \Omega(x+h,x) + O(h^{k+2}). \tag{3.48}$$

Thus, if k is odd and E is a complex line bundle, $\widehat{\Omega}^k$ is an order $k+1$ approximation to Ω.

We obtain a similar result if E is a symplectic bundle of rank 2. Recall that, if n is even, $\mathbb{C}^n$ carries a symplectic structure defined by an anti-linear map $J:\mathbb{C}^n\to\mathbb{C}^n$ of the form

$$J:\begin{pmatrix} u_1\\ u_2\\ \vdots\\ u_{n-1}\\ u_n\end{pmatrix}\mapsto\begin{pmatrix} \bar{u}_2\\ -\bar{u}_1\\ \vdots\\ \bar{u}_n\\ -\bar{u}_{n-1}\end{pmatrix}. \tag{3.49}$$

A subspace E is called symplectic if $Ju\in E$ for all $u\in E$. If E is symplectic and of rank 2, it admits an orthonormal basis of the form v^1, Jv^1. In this case, we can write the $n\times 2$ basis matrix $V=(v^1\,Jv^1)$ in the following form

$$V=\begin{pmatrix} q_1^0\mathbf{1}+q_1^1\mathbf{i}+q_1^2\mathbf{j}+q_1^3\mathbf{k}\\ \vdots\\ q_{n/2}^0\mathbf{1}+q_{n/2}^1\mathbf{i}+q_{n/2}^2\mathbf{j}+q_{n/2}^3\mathbf{k}\end{pmatrix}, \tag{3.50}$$

where q_i^μ are real and

$$\mathbf{1}=\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad \mathbf{i}=\begin{pmatrix}0&-\mathrm{i}\\-\mathrm{i}&0\end{pmatrix},\quad \mathbf{j}=\begin{pmatrix}0&-1\\1&0\end{pmatrix}\quad\text{and}\quad \mathbf{k}=\begin{pmatrix}-\mathrm{i}&0\\0&\mathrm{i}\end{pmatrix}. \tag{3.51}$$

In other words, V can be written as a vector of quaternions. It follows that each of the approximations $\Omega^k(x+h,x)$ can be written as a real linear combination of $\mathbf{1},\mathbf{i},\mathbf{j},\mathbf{k}$, and hence that

$$|\det\Omega^k(x+h,x)|^2\mathbf{1}=\Omega^k(x+h,x)\Omega^k(x+h,x)^\dagger. \tag{3.52}$$

This means that the calculation starting with equation (3.42) goes through as in the rank 1 case, and we again obtain that if k is odd, then $\widehat{\Omega}^k$ is an order $k+1$ approximation to Ω.

The final situation to consider is where E is a real rank 1 sub-bundle of a real vector bundle. This case is trivial in the sense that the parallel transport operator is a 1×1 orthogonal matrix, so is either 1 or -1. Similarly, $\widehat{\Omega}^k(x+h,x)$ has determinant ±1 so is either 1 or -1. Thus, for sufficiently small h, $\widehat{\Omega}^k$ is a perfect approximation to Ω^k.

4. Implementation

(a) Simple example

We now illustrate the methods developed earlier in a simple example. For t in the interval $[-\pi/2,\pi/2]$, let $E_t\subset\mathbb{C}^4$ be the kernel of the matrix,

$$\Gamma(t)=\begin{pmatrix}\cos t&0&\sin t&\cos t\\0&\cos t&-\cos t&\sin t\end{pmatrix}. \tag{4.1}$$

Then E is a rank 2 sub-bundle of the trivial rank 4 bundle over $[-\pi/2,\pi/2]$. We will approximate the parallel transport operator $\Omega(\pi/2,-\pi/2)$.

To do so, we choose $N+1$ equally-spaced points $t_i=-\pi/2+i\pi/N$ in the interval $[-\pi/2,\pi/2]$, with $0\le i\le N$. For each i, we find an orthonormal basis for the kernel of $\Gamma(t)$ and arrange the basis vectors into a 4×2 matrix $V(t_i)$ satisfying $V(t_i)^\dagger V(t_i)=\mathrm{Id}_2$. The kernels of $\Gamma(t_0)$ and $\Gamma(t_N)$ are equal, and for both of these, we choose the basis

$$V(t_0)=V(t_N)=\begin{pmatrix}1&0\\0&1\\0&0\\0&0\end{pmatrix}. \tag{4.2}$$

Table 1. Error in calculating the parallel transport using the methods Ω^k over N intervals.

N	6	12	24	48	96
Ω^1	3.56×10^{-1}	1.96×10^{-1}	1.03×10^{-1}	5.31×10^{-2}	2.69×10^{-2}
Ω^2	1.25×10^{-1}	3.04×10^{-2}	7.55×10^{-3}	1.88×10^{-3}	4.71×10^{-4}
Ω^3	5.61×10^{-3}	2.28×10^{-3}	3.78×10^{-4}	5.01×10^{-5}	6.36×10^{-6}
Ω^4	2.79×10^{-2}	2.23×10^{-3}	7.94×10^{-5}	3.08×10^{-6}	1.51×10^{-7}

Table 2. Error in calculating the parallel transport using the improved methods $\widehat{\Omega}^k$ over N intervals.

N	6	12	24	48	96
$\widehat{\Omega}^1$	1.23×10^{-1}	3.03×10^{-3}	7.54×10^{-3}	1.88×10^{-3}	4.71×10^{-4}
$\widehat{\Omega}^2$	1.23×10^{-1}	3.03×10^{-3}	7.54×10^{-3}	1.88×10^{-3}	4.71×10^{-4}
$\widehat{\Omega}^3$	4.30×10^{-5}	6.50×10^{-4}	4.27×10^{-5}	2.64×10^{-6}	1.65×10^{-7}
$\widehat{\Omega}^4$	9.80×10^{-3}	4.39×10^{-4}	3.52×10^{-5}	2.19×10^{-6}	1.36×10^{-7}

To approximate parallel transport to accuracy $1/N^k$, we compute the matrices $\Omega^k(t_{(i+1)(k-1)}, t_{i(k-1)})$ for $0 \leq i < N/(k-1)$. We then compute

$$U = \Omega^k(t_N, t_{N-k+1})\Omega^k(t_{N-k+1}, t_{N-2k+2}) \dots \Omega^k(t_{k-1}, t_0). \tag{4.3}$$

Our earlier results imply that $\Omega(\pi/2, -\pi/2) = U + O(1/N^k)$.

The matrix $\Omega(\pi/2, -\pi/2)$ can in fact be computed exactly by solving the differential equation (2.4). The result is

$$\Omega\left(\frac{\pi}{2}, \frac{-\pi}{2}\right) = \begin{pmatrix} -\cos\left(\frac{\pi}{\sqrt{2}}\right) & -\sin\left(\frac{\pi}{\sqrt{2}}\right) \\ \sin\left(\frac{\pi}{\sqrt{2}}\right) & -\cos\left(\frac{\pi}{\sqrt{2}}\right) \end{pmatrix}. \tag{4.4}$$

We can assess the accuracy of our approximation by computing the error $E = \frac{1}{2}\operatorname{Tr}(\Delta\Delta^\dagger)$, where $\Delta = U - \Omega(\pi/2, -\pi/2)$. The results are displayed in table 1. As expected, using a higher order method allows one to attain a desired accuracy with fewer points than would be necessary with a lower order method.

Now we consider the improved method. Recall that the improved method asks as to multiply each matrix $\Omega^k(t_{(i+1)(k-1)}, t_{i(k-1)})$ with a positive real number so that the modulus of its determinant is 1. Since scalar multiplication commutes with matrix multiplication and determinants are multiplicative, this is equivalent to computing U as in (4.3) and then computing $\widehat{U} = U/\sqrt{\det(U)}$. Thus, the additional computational cost associated with the improved method is minimal.

Nevertheless, in the cases where k is odd, the improved method $\widehat{\Omega}^k$ is a substantial improvement over Ω^k and comparable in accuracy with Ω^{k+1}, as can be seen in table 2. The reason for this improvement is that the kernel of our matrix E is a rank 2 symplectic subspace of $\mathbb{C}^4$, so by our earlier results, $\widehat{U} - \Omega(\pi/2, -\pi/2) = O(1/N^{k+1})$ when k is odd (whereas $U - \Omega(\pi/2, -\pi/2) = O(1/N^k)$).

Table 2 also shows that the errors obtained with the methods $\widehat{\Omega}^1$ and $\widehat{\Omega}^2$ are identical: this is because these two methods are in fact mathematically equivalent. To see this, one simply needs to note that

$$(V^\dagger(x)V(x+h))^{-1} = \frac{(V^\dagger(x)V(x+h))^\dagger}{|V^\dagger(x)V(x+h)|^2} = \frac{V^\dagger(x+h)V(x)}{|V^\dagger(x)V(x+h)|^2} \tag{4.5}$$

using the fact that $V^\dagger(x)V(x+h)$ can be written as a quaternion. Thus, Ω^1 and Ω^2 given in equations (2.9) and (2.23) agree up to scalar multiplication, and their normalized counterparts $\widehat{\Omega}^1$ and $\widehat{\Omega}^2$ agree exactly.

(b) Application to instantons and skyrmions

The ADHM construction produces instantons (i.e. finite-action solutions of the self-dual Yang–Mills equations) using induced connections [1–4,19]. In fact, all instantons can be produced by the ADHM method.

In the case of gauge group $SU(2)$, the method starts with an $(n+1)\times n$ matrix Δ of quaternions that depends on a point $x\in\mathbb{R}^4$. This must be written in the following form:

$$\Delta(x^1,x^2,x^3,x^4)=\begin{pmatrix} L \\ M-(x_4\mathbf{1}+x_1\mathbf{i}+x_2\mathbf{j}+x_3\mathbf{k})\otimes \mathrm{Id}_n\end{pmatrix} \tag{4.6}$$

with L, M matrices of quaternions of size $1\times n$ and $n\times n$ such that M is symmetric. The matrix must be such that $\Delta(x)^\dagger\Delta(x)$ is a real invertible matrix for all x. This constraint ensures that the kernel E_x of $\Delta(x)^\dagger$ is of quaternion dimension 1 (or complex dimension 2). So one can choose a column vector $V(x)$ of quaternions satisfying $V(x)^\dagger V(x)=\mathbf{1}$ that spans the kernel. The instanton is obtained by setting

$$A_\mu(x)=V(x)^\dagger\frac{\partial V}{\partial x^\mu}(x). \tag{4.7}$$

In other words, the instanton is the induced connection on the sub-bundle E.

Atiyah–Manton proposed [6,7] that holonomy of instantons could be used to approximate skyrmions, which are used to model atomic nuclei. To be more precise, let A be a fixed instanton with gauge group $SU(2)$. For each $(x^1,x^2,x^3)\in\mathbb{R}^3$, let $U(x^1,x^2,x^3)$ be the parallel transport operator from $t=-\infty$ to $t=\infty$ along the line in $\mathbb{R}^4$ parametrized as $t\mapsto(x^1,x^2,x^3,t)$. Atiyah–Manton proposed that the resulting function $U:\mathbb{R}^3\to SU(2)$ can be used to approximate a solution of the Euler–Lagrange equations of the Skyrme model.

This approximation was shown to work well in a number of situations [4,11–15]. Subsequently, Sutcliffe gave a theoretical explanation of the success of the approximation [16]. Sutcliffe moreover showed that instantons could also be used to approximate skyrmions coupled to vector mesons. In Sutcliffe's construction, one chooses a gauge transformation $g:\mathbb{R}^4\to SU(2)$ such that the gauge transformed connection

$$\tilde{A}_\mu=g^{-1}A_\mu g+g^{-1}\frac{\partial g}{\partial x^\mu}, \tag{4.8}$$

satisfies $A_4=0$. The vector mesons are then obtained by computing the integrals,

$$W_i(x^1,x^2,x^3)=\int_{-\infty}^{\infty}\phi(t)\tilde{A}_i(x^1,x^2,x^3,t)\,\mathrm{d}t \tag{4.9}$$

for a certain function $\phi(t)$.

Our methods provide an efficient numerical implementation of the Atiyah–Manton–Sutcliffe construction. If the ADHM data of an instanton is known, then to compute the holonomy matrix U at a point (x^1,x^2,x^3), one needs to divide the corresponding line in $\mathbb{R}^4$ into a finite number of sub-intervals. The holonomy matrix U can then be computed as a product of parallel transport operators along these intervals. To obtain accurate results, it is important to include the points $(x^1,x^2,x^3,\pm\infty)$ at the two ends of the line. The basis matrices $V(x^1,x^2,x^3,\pm\infty)$ at these two points by definition span the kernel of

$$\lim_{x^4\to\pm\infty}\frac{1}{x^4}\Delta(x^1,x^2,x^3,x^4)^\dagger=\pm\begin{pmatrix}0 & \mathbf{1}\otimes\mathrm{Id}_n\end{pmatrix}. \tag{4.10}$$

We note that the kernel of this matrix is the same in both the $+\infty$ and $-\infty$ cases and does not depend on x^1,x^2,x^3. It is important to choose the same basis $V(x^1,x^2,x^3,\pm\infty)=V_\infty$ for all values

of x^1, x^2, x^3. A very natural choice is

$$V(x^1, x^2, x^3, \pm\infty) = \begin{pmatrix} \mathbf{1} \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \tag{4.11}$$

The choice of bases at other points is of no consequence because the approximation Ω^k depends only on the choice of bases at $x^4 = \pm\infty$. The only constraint is that the columns of V should be orthonormal vectors in $\mathbb{C}^{2n+2}$.

The example described in the previous subsection corresponds to taking the holonomy of a charge 1 instanton. In this case, $n = 1$, and the ADHM matrix is particularly simple and is given by $L = \mathbf{1}$, $M = 0$. The matrix in equation (4.1) is just $\cos t \Delta^\dagger(0, 1, 0, \tan t)$, and the parallel transport operator $\Omega(\pi/2, -\pi/2)$ that we computed was therefore $U(0, 1, 0)$. Notice that our choice of parametrization $x^4 = \tan t$ maps the points $x^4 = \pm\infty$ to $t = \pm\pi/2$. This parametrization also ensures that the points on the circle in S^4 that corresponds under stereographic projection to our line in $\mathbb{R}^4$ are fairly evenly spaced. This is a sensible way to choose points because the instanton on $\mathbb{R}^4$ constructed by the ADHM construction is the pull-back of an instanton on S^4.

Our method also aids the calculation of the vector mesons. This is because the constraint $\tilde{A}_4 = 0$ imposed on the connection (4.8) is equivalent to the parallel transport equation:

$$\frac{\partial g}{\partial x^4} + A_4 g = 0. \tag{4.12}$$

One can therefore calculate $g(x^1, x^2, x^3, x^4)$ by calculating the parallel transport of A along the straight line from $(x^1, x^2, x^3, -\infty)$ to (x^1, x^2, x^3, x^4). In fact, if one was also computing U, then one would already have calculated this parallel transport as part of that process. Having calculated g, one can calculate $\tilde{A}_i$ efficiently using the identity

$$\tilde{A}_i = \tilde{V}^\dagger \frac{\partial \tilde{V}}{\partial x^i}, \quad \tilde{V} = Vg, \tag{4.13}$$

which is easily shown to be equivalent to (4.7) and (4.8). In practice, these derivatives would be approximated as finite differences. Finally, the integral in the definition (4.9) of W_i can be approximated by a finite sum.

(c) Calculating the total torsion of a space curve

In this section, we describe another possible application to the geometry of spacial curves. Let $\mathbf{x} : [0, L] \to \mathbb{R}^3$ be a smooth arclength-parametrized closed curve (meaning that $\mathbf{x}(L) = \mathbf{x}(0)$ and $d^n\mathbf{x}/\mathrm{d}s^n(L) = d^n\mathbf{x}/\mathrm{d}s^n(0)$ for all n). Let $\mathbf{u}, \mathbf{n}, \mathbf{b}$ be its Frenet frame and let κ, τ be its curvature and torsion. The total torsion of $\mathbf{x}$ is expressed as follows:

$$T := \int_0^L \tau(s)\, \mathrm{d}s. \tag{4.14}$$

This quantity appears in a number of contexts. For example, all curves embedded in a sphere have total torsion zero, and the sphere and plane are the only surfaces with this property [20]. The total torsion is a conserved quantity for the localized induction equation for vortex filaments [21] (and is the second such quantity in the hierarchy developed in [22]). The total torsion is related to the self-linking number $L \in \mathbb{Z}$ and the writhe $\mathrm{Wr} \in \mathbb{R}$ by the formula $T/2\pi = L - \mathrm{Wr}$ [23].

The torsion τ can be understood as the induced connection on the normal bundle to the curve. To see this, choose the frame $v^1(s) = \mathbf{n}(s)$ and $v^2(s) = \mathbf{b}(s)$ for the normal bundle and combine these

into a 3×2 matrix V. Then, by the Frenet equations, the induced connection is

$$A = V^{\dagger} V' = \begin{pmatrix} \mathbf{n} \cdot \mathbf{n}' & \mathbf{n} \cdot \mathbf{b}' \\ \mathbf{b} \cdot \mathbf{n}' & \mathbf{b} \cdot \mathbf{b}' \end{pmatrix} = \begin{pmatrix} 0 & -\tau \\ \tau & 0 \end{pmatrix}. \tag{4.15}$$

It follows that

$$\Omega(L, 0) = \begin{pmatrix} \cos T & \sin T \\ -\sin T & \cos T \end{pmatrix}. \tag{4.16}$$

Thus $\Omega(L, 0)$ determines the fractional part of $T/2\pi$, and of Wr.

Our methods can be used to calculate the fractional part of $T/2\pi$, and hence of Wr, to high precision. To do so with the order 3 method, one must first choose a finite set $\mathbf{x}_0, \ldots, \mathbf{x}_{2N-1}$ of points along the curve, written in the form $\mathbf{x}_i = \mathbf{x}(s_i)$ with $s_0 < s_1 < \cdots < s_{2N-1}$. Then the curve can be approximated by a polygonal arc with edge vectors $\mathbf{u}_i := \mathbf{x}_{i+1} - \mathbf{x}_i$, where the indices are understood modulo $2N$. For each edge vector, one must choose 3×2 matrices V_i satisfying $V_i^T \mathbf{u}_i = 0$ and $V_i^T V_i = \mathrm{Id}_2$. One then calculates

$$\Omega_i^2 = \frac{1}{2}(V_{i+1}^T V_i + (V_i^T V_{i+1})^{-1}), \tag{4.17}$$

$$\Omega_j^3 = \frac{4}{3}\Omega_{2j+1}^2 \Omega_{2j}^2 - \frac{1}{6}(V_{2j+2}^T V_{2j} + (V_{2j}^T V_{2j+1})^{-1}) \tag{4.18}$$

and

$$U = \Omega_{N-1}^3 \Omega_{N-2}^3 \ldots \Omega_0^3. \tag{4.19}$$

Finally, one finds an angle $\theta \in [0, 2\pi)$ by solving the system:

$$\frac{U_{11}}{\sqrt{U_{11}^2 + U_{12}^2}} = \cos\theta \quad \text{and} \quad \frac{U_{12}}{\sqrt{U_{11}^2 + U_{12}^2}} = \sin\theta. \tag{4.20}$$

The fractional part of $T/2\pi$ is given by

$$\left\lfloor \frac{T}{2\pi} \right\rfloor = \frac{\theta}{2\pi} + O\left(\frac{1}{N^3}\right). \tag{4.21}$$

Obviously, higher precision could be obtained using the order 4 method. Note that it is not necessary to choose the basis matrices V_i to approximate the Frenet frame—any choice of the orthonormal frame would be suitable because our method respects changes of basis (and because the group $SO(2)$ is abelian).

With a little more effort, one could also compute the integer part of T. To do this, one should choose the columns of V_i to be discrete approximations to the normal and binormal. For example, applying Gram–Schmidt orthogonalization to the vectors $\mathbf{u}_i, \mathbf{u}_{i+1} - \mathbf{u}_{i-1}, \mathbf{u}_i \times (\mathbf{u}_{i+1} - \mathbf{u}_{i-1})$ results in a discrete approximation to the unit tangent, normal and binormal. One then defines $H_j = \Omega_j^3 \Omega_{j-1}^3 \ldots \Omega_0^3$. One can compute the integer part of $T/2\pi$ by looking at sign changes of the upper right entry of H_j. More precisely, let n_+ be the number of integers j such that $(H_j)_{11} > 0$, $(H_j)_{12} < 0$ and $(H_{j+1})_{12} \geq 0$, and let n_- be the number of integers j such that $(H_j)_{11} > 0$, $(H_j)_{12} \geq 0$ and $(H_{j+1})_{12} < 0$. Then the total torsion is given by $T = 2\pi(n_+ - n_-) + \theta + O(N^{-3})$.

5. Conclusion

We have derived numerical methods to approximate parallel transport operators for the induced connection on a subbundle of a vector bundle. Our methods are simpler than a naive application of the Runge–Kutta method and insensitive to choices of basis.

Our most accurate method has errors of order 4. This level of accuracy should be sufficient for most applications. But the algebraic framework that we have presented could be used to derive higher order methods if desired. We expect that an order k method could be obtained for any $k \in \mathbb{N}$, and it would be of interest to find a mathematical proof of (or counterexample to) this statement.

Another interesting question concerns the number of sub-intervals required to obtain an order k method. Our order 3 method for approximating $\Omega(h, 0)$ required us to divide the interval $[0, h]$

sub-intervals of length $h/2$, while our order 4 method requires 3 sub-intervals of length $h/3$. We find it surprising that so few sub-intervals are needed. To see why, one only needs to look at equation (3.31), whose solution was required to find an order 4 method. This is a linear system of 14 equations in 4 unknowns, so it is surprising that we were able to find a solution. Similarly, the linear system (3.26) has a solution despite having more equations than unknowns. These observations suggest that there is some underlying reason why solutions can be found, despite the equations apparently being overdetermined, but we have been unable to find a satisfactory explanation. It would be an interesting mathematical problem to determine the minimum number of subdivisions required to obtain an order k method.

These questions have a natural algebraic formulation. The expressions that appear in our calculations in §3 are sums of mononomials of the form $PD^iPD^jPD^k\ldots$. These can be represented as elements $D^i\otimes D^j\otimes D^k\cdots$ of the tensor algebra $T\mathbb{R}[D]$ over the space $\mathbb{R}[D]$ of polynomials in D. In particular, the parallel transport operator $\omega(h)$ in equation (3.12) that we are trying to approximate corresponds to $\exp(-hD)=1-hD+(h^2/2)D\otimes D-\cdots$ (with h treated as a real number). This is just the exponential of $-hD$ using the tensor product. On the other hand, the expression $\pi_1(h)$ in (3.16) is $1-hD+(h^2/2)D^2-\cdots$, which is the exponential of $-hD$ defined using the polynomial product. Our approximations (3.19), (3.23) and (3.28) are Laurent polynomials in $\pi_1(nh/(k-1))$ that agree with $\omega(h)$ up to terms of total degree $k+1$. So the problem of finding approximations to the parallel transport operator amounts to comparing the exponential maps defined by two different products on $T\mathbb{R}[D]$.

Data accessibility. This article has no additional data.

Authors' contributions. D.H.: conceptualization, data curation, formal analysis, investigation, methodology, project administration, resources, software, validation, writing—original draft and writing—review and editing.

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