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CONVERGENCE ANALYSIS OF LEAPFROG FOR GEODESICS*

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Abstract. Geodesics are of fundamental interest in mathematics, physics, computer science, and many other subjects. The so-called *leapfrog algorithm* was proposed in [L. Noakes, *J. Aust. Math. Soc.,* 65 (1998), pp. 37–50] (but not named there as such) to find geodesics joining two given points x_0 and x_1 on a path-connected complete Riemannian manifold. The basic idea is to choose some junctions between x_0 and x_1 that can be joined by geodesics locally and then adjust these junctions. It was proved that the sequence of piecewise geodesics $\{\gamma^k\}_{k\geq 1}$ generated by this algorithm converges to a geodesic joining x_0 and x_1. The present paper investigates leapfrog's convergence rate $\tau_{i,n}$ of ith junction depending on the manifold M. A relationship is found with the maximal root λ_n of a polynomial of degree $n-3$, where n ($n>3$) is the number of geodesic segments. That is, the minimal $\tau_{i,n}$ is upper bounded by $\lambda_n(1+c_+)$, where c_+ is a sufficiently small positive constant depending on the curvature of the manifold M. Moreover, we show that λ_n increases as n increases. These results are illustrated by implementing leapfrog on two Riemannian manifolds: the unit 2-sphere and the manifold of all 2×2 symmetric positive definite matrices.

Key words. leapfrog, geodesics, convergence analysis, polynomial

MSC codes. 65L10, 65D15, 49J45, 53C22

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1. Introduction.

Let x_0, x_1 be given points in a smooth m-dimensional path-connected complete Riemannian manifold M. By the Hopf–Rinow theorem, x_0 and x_1 can always be joined by a (minimal) geodesic in M. Geodesics are of fundamental interest in mathematics and many other areas. In mathematics, geodesics are fundamental in studies of the geometry of a manifold, such as the Rauch comparison theorem [2] and Toponogov's triangle comparison theorem [7]. Geodesics are also essential in applications such as geodesic regression (generalized from linear regression) and principal geodesic analysis (generalized from principal component analysis), which are widely used in data analysis and computer science [6, 23, 5, 4].

When the geometric structure of the manifold M is very well understood, sometimes all geodesics can be given in closed form. Usually, however, it is necessary to determine geodesics as solutions to a 2-point boundary value problem for the $2m$-dimensional nonlinear system of geodesic equations. Initial value problems for such systems are routinely solved by numerical methods, but boundary value problems require a lot more work.

1.1. Leapfrog.

The leapfrog algorithm [15] for finding a geodesic joining $x_0, x_1 \in M$ proceeds as follows. Suppose that a piecewise geodesic $\gamma : [0,1] \to M$ from x_0 to x_1 has n geodesic segments, with any three successive junctions y_{i-1}, y_i, y_{i+1} contained in some geodesically convex subset of M. Then γ is determined by an $(n-1)$-tuple $(y_1, y_2, \ldots, y_{n-1})$ of junctions, and we set $y_0 := x_0$ and $y_n := x_1$. Then, for

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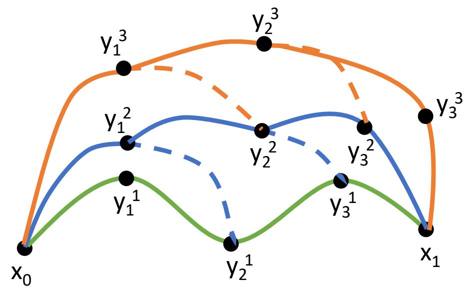

Fig. 1. *An illustration of leapfrog for 3 junctions: choose 3 initial junctions y_1^1, y_2^1, and y_3^1; then y_1^1 is moved to the midpoint y_1^2 of the minimal geodesic joining x_0 and y_2^1, y_2^1 is moved to the midpoint y_2^2 of the minimal geodesic joining y_1^2 and y_3^1, and y_3^1 is moved to the midpoint y_3^2 of the minimal geodesic joining y_2^2 and x_1. This process continues unless some stop criterion is satisfied.*

$i = 1, 2, \ldots, n-1$, y_i is adjusted by moving y_i onto the midpoint of the minimal geodesic joining y_{i-1} and y_{i+1}, as in Figure 1.

This generates a sequence of piecewise geodesic curves $\Omega = \{\gamma^k : [0,1] \to N, k \geq 1\}$. Denoting the ith junction of γ^k by y_i^k, with $y_0^k = x_0$ and $y_n^k = x_1$, y_i^k is the midpoint of the minimal geodesic joining y_{i-1}^k and y_{i+1}^{k-1}. As proved in [15] the limits $y_i^\infty := \lim_{k\to\infty} y_i^k$ almost always exist, and these allow us to construct a geodesic γ^∞ from x_0 to x_1. The number n of geodesic segments is determined by the effectiveness of methods to find geodesics joining y_{i-1}^k and y_{i+1}^{k-1}. Usually this is done by single shooting, which works well if a good initial guess can be made for the initial velocity of the geodesic. For instance, when n is moderately large, consecutive junctions need not be too far apart. Then good linear estimates can be made using coordinate charts.

Regarding the endpoint geodesic problem, Bryner in [1] proposed two numerical schemes, the shooting method and path-straightening, to compute endpoint geodesics on Stiefel manifolds by considering them as submanifolds of the Euclidean space. From the perspective of matrix-algebra, Zimmermann in [26] derived a method for evaluating the Riemannian logarithm map on the Stiefel manifold with respect to the canonical metric. Later, Zimmermann and Hüper in [27] provided a unified method to deal with the geodesic endpoint problem on the Stiefel manifold with respect to a family of metrics. In [22], Sutti and Vandereycken discussed the convergence of the leapfrog algorithm as a nonlinear Gauss–Seidel method on the Stiefel manifold.

Recently the present authors proposed an alternative algorithm to find geodesics joining two given points [18]. Like leapfrog, this method also exploits single shooting to find geodesics joining junctions. The key difference is in the way that junctions are adjusted, and there does not seem to be much difference in performance of the two methods (if anything, leapfrog is preferable). Leapfrog has also been adapted to find optimal trajectories in optimal control problems [8, 9].

Apart from the applications mentioned above, leapfrog is also used for finding extremals of Lagrangian actions [19] in physics, where the Lagrange mechanic systems may include double pendulum, obstacle avoidance, and navigation problems, to name a few. In data science, for the problem of fitting multidimensional reduced data, leapfrog can work as an iterative scheme that selects the missing knots by minimizing a nonlinear multivariate function [10, 11]. In computer vision, a 2D version of leapfrog is proposed to recover an unknown surface from 3 noisy camera images [17] and applied to photometric stereo reconstruction [16]. In engineering, the leapfrog method is shown to produce optimal paths of a mobile robot by solving some nonlinear equations [13, 14]. In finance, many real-world problems are too complicated to lead to analytical solutions; computational algorithms including leapfrog are essential tools for dynamic optimizations in modeling economic growth [3].

In [15] it is shown that the sequence of piecewise geodesics $\{\gamma^k\}_{k\geq 1}$ generated by leapfrog almost always converges to a geodesic joining x_0 and x_1 (there is always a subsequence that converges to a geodesic). However, there has been no study of convergence rates

$$\tau_{i,n} := \lim_{k\to\infty} \frac{d(y_i^{k+1}, y_i^{\infty})}{d(y_i^k, y_i^{\infty})},$$

where $d : M \times M \to \mathbb{R}$ is the Riemannian distance. In practice, the $\tau_{i,n}$ seem to increase dramatically with n (it is a mistake to choose n unnecessarily large). In Theorem 2.4, we present an upper bound for the convergence rate of the L_∞ norm of the vector of errors at all junctions, which may imply an upper bound for $\tau_{i,n}$ but not very tight.

To state our main result, we introduce, for variable s,

$$p_n(s) := \frac{1}{\mu_+ - \mu_-}\left[16\left(\mu_+^{n-2} - \mu_-^{n-2}\right) - 8\left(\mu_+^{n-3} - \mu_-^{n-3}\right) + \left(\mu_+^{n-4} - \mu_-^{n-4}\right)\right],$$

where $\mu_\pm = \frac{s\pm\sqrt{s^2-s}}{2}$. It will turn out that $p_n(s)$ is a polynomial in s with real roots when $n \geq 4$ (see Lemma 3.4). The central result of the present paper is given as follows.

THEOREM 3.1. *Suppose every three consecutive junctions in the leapfrog algorithm are sufficiently close, the sectional curvature of the manifold M is bounded, and λ_n is the largest root of the polynomial $p_n(s)$. Then, there exists a sufficient small positive constant $c_+ \in [0,1)$ such that*

$$\tau_n^- := \min_{2\leq i\leq n-1} \tau_{i,n} \leq \lambda_n(1 + c_+).$$

Moreover, $c_+ = 0$ if M has nonpositive sectional curvature.

The paper is organized as follows. In section 2, we present some local analysis on the junctions, i.e., the relationship between $d(y_i^{k+1}, y_i^\infty)$, $d(y_{i-1}^{k+1}, y_{i-1}^\infty)$, and $d(y_{i+1}^k, y_{i+1}^\infty)$. Then we study convergence rates of leapfrog for $n = 3, 4, 5$, preparatory to the remaining cases where $n \geq 6$ in section 3. In section 3 we present some properties of the polynomial $p_n(s)$ including the recurrence relationship and real roots of $p_n(s)$. The proof of Theorem 3.1 is given in section 4. In section 5, we illustrate our results by using leapfrog to find geodesics joining given points in the unit 2-sphere and in the manifold of all 2×2 symmetric positive definite matrices. A conclusion is given in section 6.

2. Convergence rates for few junctions.

In this section, we investigate convergence rates of leapfrog when the number $n-1$ of junctions is $2, 3, 4$. As a key building block, we firstly study the relationship between $d(y_i^{k+1}, y_i^\infty)$, $d(y_{i-1}^{k+1}, y_{i-1}^\infty)$, and $d(y_{i+1}^k, y_{i+1}^\infty)$.

Working in normal coordinates about x_0 (which we always do from now on), Theorem 5.1 in [15] says that a subsequence of $\{\gamma^k : [0,1] \to M\}_{k\geq 1}$ converges to the geodesic $\gamma^\infty(t) = tx_1$. Assuming that the subsequence is the whole sequence (as shown in [15] for most circumstances), the junctions y_i^k on γ^k converge to $y_i^\infty = \frac{i}{n}x_1$ on γ^∞. So by starting with k sufficiently large, we may suppose that, for some small $\delta > 0$,

$$e_i^k := d(y_i^k, y_i^\infty) = \mathcal{O}(\delta), \tag{2.1}$$

where $d : M \times M \to \mathbb{R}$ is the Riemannian distance function. Evidently $e_0^k = e_n^k = 0$.

From now on, we suppose every three consecutive junctions in the leapfrog algorithm are sufficiently close for the convenience of constructing our convergence theory. Note that the two given endpoints are not close in general.

2.1. Local analysis. For the purpose of analyzing the local relationship between e_i^{k+1}, e_{i-1}^{k+1}, and e_{i+1}^k, we need to estimate the geodesic distance e_i^k up to certain order of δ. The following useful lemma is taken from [12] (see Lemma 4.3.3 there).

LEMMA 2.1. *Let M be a complete Riemannian manifold with a Riemannian metric $\langle\cdot,\cdot\rangle$, $(\mathcal{U}, (x^i))$ any normal coordinate chart centered at $s \in M$. If two points p and q are sufficiently close to s, then the square of the geodesic distance $d^2(p,q)$ can be written as*

$$d^2(p,q) = \|p-q\|^2 - \frac{1}{3}\langle R(q,p)p, q\rangle + \mathcal{O}\left(\|p-q\|^4\right),$$

where $\|\cdot\|$ is the standard Euclidean norm, $\langle R(q,p)p,q\rangle := \langle R(\overrightarrow{sq}, \overrightarrow{sp})\overrightarrow{sp}, \overrightarrow{sq}\rangle$, $\overrightarrow{sp}$ and $\overrightarrow{sq}$ are tangent vectors in normal coordinates, and R is the Riemannian curvature tensor on M.

Note that the term $\langle R(q,p)p,q\rangle$ can be rewritten in terms of sectional curvature, i.e.,

$$\langle R(q,p)p,q\rangle = K(p,q)\cdot\left(\|p\|^2\|q\|^2 - \langle p,q\rangle^2\right),$$

where $K(p,q)$ is the sectional curvature and the Riemannian norm/metric is the same as the Euclidean one since normal coordinates are chosen at s.

LEMMA 2.2. *Let M be a complete Riemannian manifold, $\triangle xyz$ a geodesic triangle in M (a triangle each of whose sides is a minimal geodesic), and p and q the midpoints of the geodesics xy and xz, respectively. Suppose $\triangle xyz$ is sufficiently small and $d(p,q) = \mathcal{O}(\delta) = d(y,z)$; then there exist two sufficiently small positive constants c_- and c_+ such that*

$$\frac{1}{2}\sqrt{1-c_-}\,d(y,z) \le d(p,q) \le \frac{1}{2}\sqrt{1+c_+}\,d(y,z). \tag{2.2}$$

Moreover, $c_+ = 0$ ($c_- = 0$) if M has nonpositive (nonnegative) sectional curvature.

To increase the readability of this paper, we put the proof of Lemma 2.2 in Appendix A.

LEMMA 2.3. *For sufficiently large k, $i = 1, 2, \ldots, n-1$, the geodesic distances e_i^{k+1}, e_{i-1}^{k+1}, and e_{i+1}^k satisfy the following relationship:*

$$e_i^{k+1} \le \frac{1}{2}\sqrt{1+c_+}\left(e_{i-1}^{k+1} + e_{i+1}^k\right), \tag{2.3}$$

where $c_+ \in [0,1)$ is some constant. Further, $c_+ = 0$ if M has nonpositive sectional curvature.

Refer to Appendix B for the proof of Lemma 2.3. For simplicity, we denote $\kappa := \frac{1}{2}\sqrt{1+c_+}$ and $\underline{\kappa} := \frac{1}{2}\sqrt{1-c_-}$ from now on.

If we view the errors $(e_2^k, e_3^k, \ldots, e_{n-1}^k)$ as a vector v^k in $\mathbb{R}^{n-2}$, then the convergence rate of the L_∞ norm of v^k is upper bounded.

THEOREM 2.4. *Let τ_∞ be the convergence rate of the L_∞ norm of the error vector $v^k := (e_2^k, e_3^k, \ldots, e_{n-1}^k)$; we have*

$$\tau_\infty = \lim_{k\to\infty} \frac{\|v^{k+1}\|_\infty}{\|v^k\|_\infty} \le \frac{\kappa(1-\kappa^{n-2})}{1-\kappa}. \tag{2.4}$$

Refer to Appendix C for the proof of Theorem 2.4. In what follows, we will consider the convergence rate of $\{\gamma^k\}$ for small number of junctions by taking advantage of Lemmas 2.2 and 2.3.

2.2. Analysis for $n = 3$. We start with the simplest case where $n = 3$, i.e., initial junctions (y_1^1, y_2^1) are given.

THEOREM 2.5. *The convergence rates of y_1^k, y_2^k to y_1^∞, y_2^∞ are upper bounded by $\frac{1}{4}(1 + c_+)$ and lower bounded by $\frac{1}{4}(1 - c_-)$. Moreover, $c_+ = 0$ ($c_- = 0$) if M has nonpositive (nonnegative) sectional curvature.*

Proof. By Lemma 2.2, we have

$$\underline{\kappa} e_2^k \le e_1^{k+1} \le \kappa e_2^k, \tag{2.5}$$

$$\underline{\kappa} e_1^{k+1} \le e_2^{k+1} \le \kappa e_1^{k+1}. \tag{2.6}$$

Substituting (2.5) into (2.6) results in

$$\underline{\kappa}^2 e_2^k \le e_2^{k+1} \le \kappa^2 e_2^k.$$

Substituting (2.6) into (2.5) results in

$$\underline{\kappa}^2 e_1^k \le e_1^{k+1} \le \kappa^2 e_1^k.$$

Therefore, the convergence rate of y_i^k is given by

$$\tau_{i,3} = \lim_{k\to\infty} \frac{e_i^{k+1}}{e_i^k} \in \left[\underline{\kappa}^2, \kappa^2\right], \tag{2.7}$$

where $i = 1, 2$. ∎

Note that if there exists a k_0 such that $e_i^k = 0$ for $k > k_0$, there is no sense in discussing the limitation $\lim_{k\to\infty} \frac{e_i^{k+1}}{e_i^k}$.

2.3. Analysis for $n = 4$. Suppose 3 junctions (y_1^1, y_2^1, y_3^1) are given.

THEOREM 2.6. *For $n = 4$, we have the following estimation:*

$$\tau_{2,4} \le \frac{1}{2}(1 + c_+), \quad \tau_4^- \le \frac{1}{2}(1 + c_+).$$

Moreover, $c_+ = 0$ if M has nonpositive sectional curvature.

Proof. By Lemma 2.3, we have

$$e_1^{k+1} \le \kappa e_2^k, \tag{2.8}$$

$$e_2^{k+1} \le \kappa \left(e_1^{k+1} + e_3^k\right), \tag{2.9}$$

$$e_3^{k+1} \le \kappa e_2^{k+1}. \tag{2.10}$$

Substituting (2.8) and (2.10) into (2.9) yields

$$e_2^{k+1} \le 2\kappa^2 e_2^k, \tag{2.11}$$

which implies $\tau_{2,4} \le 2\kappa^2$. Then $\tau_4^- \le 2\kappa^2$ follows directly. Alternatively, we can consider the linear combination $2\kappa\times$(2.8) $+2\times$(2.9) + (2.10)/κ, i.e.,

$$e_2^{k+1} + \frac{e_3^{k+1}}{\kappa} \le 2\kappa^2 \left(e_2^k + \frac{e_3^k}{\kappa} \right), \tag{2.12}$$

which indicates

$$\tau_4^- \le \lim_{k\to\infty} \frac{e_2^{k+1} + \frac{e_3^{k+1}}{\kappa}}{e_2^k + \frac{e_3^k}{\kappa}} \le 2\kappa^2. \tag{2.13}$$

□

In general, the convergence rates $\tau_{1,n}$ and $\tau_{2,n}$ are close, so are $\tau_{n-2,n}$ and $\tau_{n-1,n}$. This is because

$$\frac{\underline{\kappa} e_2^k}{\kappa e_2^{k-1}} \le \frac{e_1^{k+1}}{e_1^k} \le \frac{\kappa e_2^k}{\underline{\kappa} e_2^{k-1}} \implies \underline{c}\tau_{2,n} \le \tau_{1,n} \le \bar{c}\tau_{2,n},$$
$$\frac{\underline{\kappa} e_{n-2}^{k+1}}{\kappa e_{n-2}^k} \le \frac{e_{n-1}^{k+1}}{e_{n-1}^k} \le \frac{\kappa e_{n-2}^{k+1}}{\underline{\kappa} e_2^k} \implies \underline{c}\tau_{n-2,n} \le \tau_{n-1,n} \le \bar{c}\tau_{n-2,n},$$

where $\underline{c} = \frac{\underline{\kappa}}{\kappa} = \sqrt{\frac{1-c_-}{1+c_+}}$ and $\bar{c} = \frac{\kappa}{\underline{\kappa}} = \sqrt{\frac{1+c_+}{1-c_-}}$ are close to 1.

2.4. Analysis for $n = 5$. Suppose 4 junctions $(y_1^1, y_2^1, y_3^1, y_4^1)$ are given.

THEOREM 2.7. *For $n = 5$, we have the following estimation:*

$$\tau_5^- \le \frac{3+\sqrt{5}}{8}(1+c_+).$$

Moreover, $c_+ = 0$ if M has nonpositive sectional curvature.

Proof. By Lemma 2.3, we have

$$e_1^{k+1} \le \kappa e_2^k, \tag{2.14}$$
$$e_2^{k+1} \le \kappa \left(e_1^{k+1} + e_3^k \right), \tag{2.15}$$
$$e_3^{k+1} \le \kappa \left(e_2^{k+1} + e_4^k \right), \tag{2.16}$$
$$e_4^{k+1} \le \kappa e_3^{k+1}. \tag{2.17}$$

Considering the linear combination $\kappa(1+\kappa a_2)\times$ (2.14) $+(1+\kappa a_2)\times$ (2.15) $+a_2\times$ (2.16) $+a_3\times$ (2.17) $(a_2, a_3 > 0)$, one has

$$e_2^{k+1} + (a_2 - \kappa a_3) e_3^{k+1} + a_3 e_4^{k+1} \le \kappa^2 (1+\kappa a_2) e_2^k + \kappa (1+\kappa a_2) e_3^k + \kappa a_2 e_4^k.$$

We let

$$\begin{cases} \kappa^2 (1+\kappa a_2)(a_2 - \kappa a_3) = \kappa (1+\kappa a_2), \\ \kappa^2 (1+\kappa a_2) a_3 = \kappa a_2, \end{cases}$$
$$\implies \begin{cases} a_2 = \frac{1\pm\sqrt{5}}{2\kappa}, \\ a_3 = \frac{-1\pm\sqrt{5}}{2\kappa^2}. \end{cases}$$

Therefore, choosing positive a_2 and a_3, we find

$$e_2^{k+1} + \frac{e_3^{k+1}}{\kappa} + \frac{\sqrt{5}-1}{2\kappa^2} e_4^{k+1} \leq \frac{3+\sqrt{5}}{2}\kappa^2 \left(e_2^k + \frac{e_3^k}{\kappa} + \frac{\sqrt{5}-1}{2\kappa^2} e_4^k \right),$$

which means

$$\tau_5^- \leq \lim_{k\to\infty} \frac{e_2^{k+1} + \frac{e_3^{k+1}}{\kappa} + \frac{\sqrt{5}-1}{2\kappa^2} e_4^{k+1}}{e_2^k + \frac{e_3^k}{\kappa} + \frac{\sqrt{5}-1}{2\kappa^2} e_4^k} \leq \frac{3+\sqrt{5}}{2}\kappa^2. \tag{2.18}$$ ∎

From the above three cases, we observe that if we can get a recurrence relationship involving linear combinations of e_i^{k+1} and those of e_i^k, it is possible to estimate the upper bound of the convergence rate of leapfrog. In other words, we analyze the convergence rate of some sort of norm of the error vector $(e_2^k, e_3^k, \ldots, e_{n-1}^k)$. Note that Theorem 2.4 evaluates the convergence rate of the L_∞ norm of the error vector, where the upper bound may not be very tight. With this motivation in mind and following the strategy used in the cases with few junctions, we will discuss how to determine the coefficients of the linear combination in the general case in the following section.

3. Convergence rates for remaining cases. We now consider the remaining cases, where $n \geq 6$.

THEOREM 3.1. *Suppose every three consecutive junctions in the leapfrog algorithm are sufficiently close, and the sectional curvature of the manifold M is bounded. For $i = 1, \ldots, n-1$, let $\tau_{i,n}$ be the convergence rate of y_i^k to y_i^∞, i.e.,*

$$\tau_{i,n} = \lim_{k\to\infty} \frac{e_i^{k+1}}{e_i^k} = \lim_{k\to\infty} \frac{d(y_i^{k+1}, y_i^\infty)}{d(y_i^k, y_i^\infty)}.$$

Suppose λ_n is the largest root of the following polynomial:

$$p_n(s) = \frac{1}{\mu_+ - \mu_-}\left[16\left(\mu_+^{n-2} - \mu_-^{n-2}\right) - 8\left(\mu_+^{n-3} - \mu_-^{n-3}\right) + \left(\mu_+^{n-4} - \mu_-^{n-4}\right)\right], \tag{3.1}$$

where $\mu_\pm = \frac{s \pm \sqrt{s^2 - s}}{2}$. Then, there exists a sufficiently small positive constant $c_+ \in [0, 1)$ such that

$$\tau_n^- := \min_{2\leq i\leq n-1} \tau_{i,n} \leq \lambda_n(1 + c_+).$$

Moreover, $c_+ = 0$ if M has nonpositive sectional curvature.

The proof of Theorem 3.1 is delayed until section 4. Here we discuss some properties of the polynomial $p_n(s)$.

Remark 3.2. Theorem 3.1 can be verified for $n = 3, 4, 5$ by the following calculations:

$$p_3(s) = 16 - \frac{4}{s} = 0 \implies s = \frac{1}{4},$$
$$p_4(s) = 16s - 8 = 0 \implies s = \frac{1}{2},$$
$$p_5(s) = 16s^2 - 12s + 1 = 0 \implies s = \frac{3 \pm \sqrt{5}}{8},$$

which is consistent with Theorems 2.5, 2.6, 2.7.

Remark 3.3. By the formula

$$\mu_+^n - \mu_-^n = (\mu_+ - \mu_-)\left(\mu_+^{n-1} + \mu_+^{n-2}\mu_- + \cdots + \mu_+\mu_-^{n-2} + \mu_-^{n-1}\right),$$

(3.1) can be rewritten as

$$p_n(s) = 16\sum_{i=0}^{n-3}\mu_+^{n-3-i}\mu_-^i - 8\sum_{i=0}^{n-4}\mu_+^{n-4-i}\mu_-^i + \sum_{i=0}^{n-5}\mu_+^{n-5-i}\mu_-^i. \tag{3.2}$$

It seems not so straightforward that we can view $p_n(s)$ $(n \geq 4)$ as a polynomial. Readers may doubt whether all roots of $p_n(s)$ are real and located in $[0,1)$. The following lemma makes an effort to answer these questions and study its broader properties.

Lemma 3.4.

(1) *For $n \geq 5$, $p_n(s)$ satisfies the following recurrence relationship:*

$$p_n(s) = sp_{n-1}(s) - \frac{1}{4}sp_{n-2}(s), \tag{3.3}$$

which means $p_n(s)$ is a polynomial with real coefficients.

(2) *$p_n(s)$ $(n \geq 4)$ is a polynomial of degree $n-3$ and the coefficient of s^{n-3} (known as the leading coefficient) is 16. The smallest power of s in $p_n(s)$ is $\lfloor \frac{n}{2} \rfloor - 2$ and its coefficient is $k(-\frac{1}{4})^{k-3}$ if $n = 2k$, $(-\frac{1}{4})^{k-2}$ if $n = 2k+1$. That is,*

$$p_n(s) = \begin{cases} 16s^{2k-3} + \displaystyle\sum_{j=k-1}^{2k-4} a_j^n s^j + k\left(-\frac{1}{4}\right)^{k-3} s^{k-2}, & n = 2k, \\ 16s^{2k-2} + \displaystyle\sum_{j=k-1}^{2k-3} a_j^n s^j + \left(-\frac{1}{4}\right)^{k-2} s^{k-2}, & n = 2k+1, \end{cases} \tag{3.4}$$

where a_j^n's are some real numbers.

(3) *0 is a root of $p_n(s)$ $(n \geq 6)$ with multiplicity $\lfloor \frac{n}{2} \rfloor - 2$; i.e., there exists a polynomial $q_n(s)$ of degree $\lceil \frac{n}{2} \rceil - 1$ such that*

$$p_n(s) = s^{\lfloor \frac{n}{2} \rfloor - 2} q_n(s), \tag{3.5}$$

where $0 \neq q_n(0) = (\lfloor \frac{n}{2} \rfloor)^{\frac{1+(-1)^n}{2}} (-\frac{1}{4})^{\lceil \frac{n}{2} \rceil - 3}$.

(4) *For $n \geq 6$, $q_n(s)$ satisfies the following recurrence relationship:*

$$q_n(s) = s^{\frac{1-(-1)^n}{2}} q_{n-1} - \frac{1}{4} q_{n-2}(s). \tag{3.6}$$

(5) *$q_n(s)$ $(n \geq 6)$ has $\lceil \frac{n}{2} \rceil - 1$ distinct real roots.*

(6) *For $n \geq 3$, all roots of the polynomial $p_n(s)$ are real and located in $[0,1)$, which means the largest root of $p_n(s)$ belongs to $(0,1)$.*

Proof. (1) By (3.2), we have

$$\begin{aligned} p_n(s) &= \mu_+ p_{n-1}(s) + 16\mu_-^{n-3} - 8\mu_-^{n-4} + \mu_-^{n-5} \\ &= \mu_- p_{n-1}(s) + 16\mu_+^{n-3} - 8\mu_+^{n-4} + \mu_+^{n-5}, \end{aligned}$$

which implies

$$p_n(s) = \frac{1}{2}sp_{n-1}(s) + 8(\mu_+^{n-3} + \mu_-^{n-3}) - 4(\mu_+^{n-4} + \mu_-^{n-4}) + \frac{1}{2}(\mu_+^{n-5} + \mu_-^{n-5}). \tag{3.7}$$

Again, by (3.2),

$$p_n(s) = \frac{1}{4}sp_{n-2}(s) + 16(\mu_+^{n-3} + \mu_-^{n-3}) - 8(\mu_+^{n-4} + \mu_-^{n-4}) + \mu_+^{n-5} + \mu_-^{n-5}. \tag{3.8}$$

Therefore, 2×(3.7)–(3.8) gives the recurrence relationship (3.3).

(2) By Remark 3.2, (3.4) holds for $n = 4$ and $n = 5$. Suppose (3.4) is true for $n = 4, 5, \ldots, m$. Now we consider the case where $n = m + 1$.

(i) If $m = 2k$, then

$$\begin{aligned} p_{m+1}(s) &= sp_m(s) - \frac{1}{4}sp_{m-1}(s) \\ &= s\left(16s^{2k-3} + \cdots + k\left(-\frac{1}{4}\right)^{k-3} s^{k-2}\right) \\ &\quad - \frac{1}{4}s\left(16s^{2k-4} + \cdots + \left(-\frac{1}{4}\right)^{k-3} s^{k-3}\right) \\ &= 16s^{2k-2} + \cdots + \left(-\frac{1}{4}\right)^{k-2} s^{k-2}. \end{aligned}$$

(ii) If $m = 2k + 1$, then

$$\begin{aligned} p_{m+1}(s) &= sp_m(s) - \frac{1}{4}sp_{m-1}(s) \\ &= s\left(16s^{2k-2} + \cdots + \left(-\frac{1}{4}\right)^{k-2} s^{k-2}\right) \\ &\quad - \frac{1}{4}s\left(16s^{2k-3} + \cdots + k\left(-\frac{1}{4}\right)^{k-3} s^{k-2}\right) \\ &= 16s^{2k-1} + \cdots + (k+1)\left(-\frac{1}{4}\right)^{k-2} s^{k-1}, \end{aligned}$$

which completes this proof by induction.

(3) (3.5) follows from (3.4) directly.

(4) By (3.3) and (3.5),

$$\begin{aligned} q_{2k}(s) &= q_{2k-1}(s) - \frac{1}{4}q_{2k-2}(s), \\ q_{2k+1}(s) &= sq_{2k}(s) - \frac{1}{4}q_{2k-1}(s), \end{aligned}$$

which implies (3.6).

(5) We put the lengthy proof in Appendix D.

(6) It is sufficient to prove that when $n \geq 6$, $p_n(s) \neq 0$ for $s \geq 1$ or $s < 0$.

(i) If $s = 1$, then

$$p_n(s) = 16(n-4)\frac{1}{2^{n-3}} - 8(n-3)\frac{1}{2^{n-4}} + (n-4)\frac{1}{2^{n-5}} = \frac{n}{2^{n-5}} > 0.$$

(ii) If $s > 1$, then $\mu_+ > \mu_- > 0$ and $\mu_+ > \frac{1}{2}$. Thus, we have

$$\frac{16(\mu_+^{n-2} - \mu_-^{n-2})}{8(\mu_+^{n-2} - \mu_-^{n-2})} = 2\mu_+ \frac{1 - (\frac{\mu_-}{\mu_+})^{n-2}}{1 - (\frac{\mu_-}{\mu_+})^{n-3}} > 2\mu_+ > 1,$$

which means $p_n(s) > 0$.

(iii) If $s<0$, then $0<\mu_+<-\mu_-$, which implies

$$\mu_+^k-\mu_-^k=\begin{cases}\mu_+^k-(-\mu_-)^k<0, & k \text{ is even},\\ \mu_+^k+(-\mu_-)^k>0, & k \text{ is odd}.\end{cases}$$

Therefore, we find

$$\begin{aligned}p_n(s)&=\frac{1}{\mu_+-\mu_-}\left[16(\mu_+^{n-2}-\mu_-^{n-2})-8(\mu_+^{n-3}-\mu_-^{n-3})+(\mu_+^{n-4}-\mu_-^{n-4})\right]\\&=\begin{cases}<0, & n \text{ is even},\\ >0, & n \text{ is odd},\end{cases}\end{aligned}$$

which completes this proof. ∎

Figure 2 shows the polynomial $p_n(s)$ and its largest root for $6\le n\le 10$, from which we can observe that the larger the n value, the larger the largest root of $p_n(s)$.

THEOREM 3.5. *Let λ_n,λ_{n-1} be the largest roots of $p_n(s)$ and $p_{n-1}(s)$, respectively; then*

$$\lambda_n>\lambda_{n-1}. \tag{3.9}$$

Proof. We prove this theorem by induction on n. By Remark 3.2, we know $\lambda_5>\lambda_4>\lambda_3>0$.

Suppose $\lambda_n>\lambda_{n-1}$ holds for $n=k$; now we need to prove $\lambda_{k+1}>\lambda_k$. Suppose $\lambda_{k+1}\le\lambda_k$. By (3.3),

$$p_{k+1}(\lambda_k)=\lambda_k p_k(\lambda_k)-\frac{1}{4}\lambda_k p_{k-1}(\lambda_k)=-\frac{1}{4}\lambda_k p_{k-1}(\lambda_k)<0,$$

where we have used the relation $p_{k-1}(\lambda_k)>p_{k-1}(\lambda_{k-1})=0$. Note that $p_n(s)$ is increasing on $[\lambda_n,+\infty)$. Therefore, we get

$$p_{k+1}(\lambda_k)<0=p_{k+1}(\lambda_{k+1})\implies\lambda_k<\lambda_{k+1}, \tag{3.10}$$

which contradicts our assumption. ∎

Remark 3.6. For $s\in(0,1)$, the polynomial $p_n(s)$ tends to the null polynomial $p_n(s)\equiv 0$ as $n\to\infty$, whose largest root disappears.

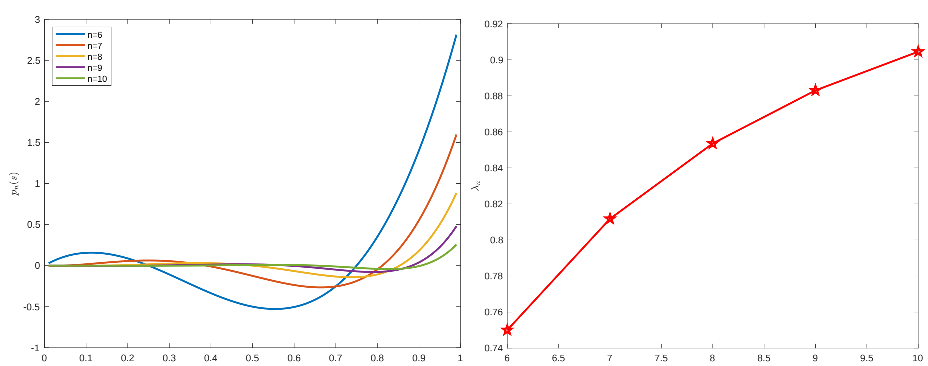

FIG. 2. *The polynomial $p_n(s)$ (left) and its largest root (right) for $n=6,\dots,10$.*

4. Proof of Theorem 3.1. The main purpose of this section is to prove Theorem 3.1, and we focus on $\tau_n^- \leq \lambda_n(1+c_+)$.

By Lemma 2.3, we have

$$e_1^{k+1} \leq \kappa e_2^k, \tag{4.1}$$

$$e_2^{k+1} \leq \kappa\left(e_1^{k+1} + e_3^k\right), \tag{4.2}$$

$$e_3^{k+1} \leq \kappa\left(e_2^{k+1} + e_4^k\right), \tag{4.3}$$

$$\cdots$$

$$e_{n-1}^{k+1} \leq \kappa e_{n-2}^{k+1}. \tag{4.4}$$

Similar to the proof of Theorem 2.7, we consider the linear combinations $\kappa(1+\kappa a_2)\times$ (4.1) + $(1+\kappa a_2)\times$(4.2) + $a_2\times$(4.3) + $\cdots + a_{n-2}\times$(4.4) ($a_i > 0, i = 2, \ldots, n-2$),

$$\begin{aligned} &e_2^{k+1} + (a_2 - \kappa a_3)e_3^{k+1} + (a_3 - \kappa a_4)e_4^{k+1} + \cdots + (a_{n-3} - \kappa a_{n-2})e_{n-2}^{k+1} + a_{n-2}e_{n-1}^{k+1} \\ &\leq \kappa^2(1+\kappa a_2)e_2^k + \kappa(1+\kappa a_2)e_3^k + \kappa a_2 e_4^k + \cdots + \kappa a_{n-4}e_{n-2}^k + \kappa a_{n-3}e_{n-1}^k. \end{aligned}$$

We let

$$\begin{cases} \kappa^2(1+\kappa a_2)(a_2 - \kappa a_3) = \kappa(1+\kappa a_2), \\ \kappa^2(1+\kappa a_2)(a_3 - \kappa a_4) = \kappa a_2, \\ \cdots \\ \kappa^2(1+\kappa a_2)(a_{n-3} - \kappa a_{n-2}) = \kappa a_{n-4}, \\ \kappa^2(1+\kappa a_2)a_{n-2} = \kappa a_{n-3}. \end{cases} \tag{4.5}$$

Define $a_1 = \kappa^2(1+\kappa a_2)$; then (4.5) can be rewritten as

$$\mathbf{A}\mathbf{a} = \mathbf{c}, \tag{4.6}$$

where

$$\mathbf{A} = \begin{bmatrix} 1 & -\kappa^3 & & & & & \\ & 1 & -\kappa & & & & \\ & -\kappa & a_1 & -\kappa a_1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -\kappa & a_1 & -\kappa a_1 \\ & & & & -\kappa & a_1 \end{bmatrix}, \mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_{n-3} \\ a_{n-2} \end{bmatrix}, \mathbf{c} = \begin{bmatrix} \kappa^2 \\ \kappa^{-1} \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix},$$

which means

$$a_1 = \kappa^2(\mathbf{A}^{-1})_{11} + \kappa^{-1}(\mathbf{A}^{-1})_{12}, \tag{4.7}$$

where $(\mathbf{A}^{-1})_{ij}$ is the (i,j)th element of the matrix $\mathbf{A}^{-1}$. Note that $a_1 = \kappa^2(1+\kappa a_2) > \kappa^2$; thus, $\mathbf{A}^{-1}$ in (4.7) is meaningful.

Recall the following formula [24, equation (4.13)]: The inverse of a nonsingular tridiagonal matrix T,

$$T = \begin{bmatrix} d_1 & b_1 & & & \\ c_1 & d_2 & b_2 & & \\ & c_2 & \ddots & \ddots & \\ & & \ddots & \ddots & b_{m-1} \\ & & & c_{m-1} & d_m \end{bmatrix},$$

is given by

$$(T^{-1})_{ij} = \begin{cases} (-1)^{i+j} b_i \cdots b_{j-1} \theta_{i-1} \phi_{j+1}/\theta_m & \text{if } i < j, \\ \theta_{i-1}\phi_{j+1}/\theta_m & \text{if } i = j, \\ (-1)^{i+j} c_j \cdots c_{i-1} \theta_{j-1} \phi_{i+1}/\theta_m & \text{if } i > j, \end{cases}$$

where the θ_i satisfy the recurrence relation

$$\theta_i = d_i \theta_{i-1} - b_{i-1} c_{i-1} \theta_{i-2}, \quad i = 2, 3, \ldots, m,$$

with initial conditions $\theta_0 = 1, \theta_1 = d_1$, and the ϕ_i satisfy

$$\phi_i = d_i \phi_{i+1} - b_i c_i \phi_{i+2}, \quad i = m-1, m-2, \ldots, 1,$$

with initial conditions $\phi_{m+1} = 1$ and $\phi_m = d_m$.

In our case,

$$b_i = \begin{cases} -\kappa^3, & i = 1, \\ -\kappa, & i = 2, \\ -\kappa a_1, & 3 \leq i \leq n-3, \end{cases} \quad c_i = \begin{cases} 0, & i = 1, \\ -\kappa, & 2 \leq i \leq n-3, \end{cases} \quad d_i = \begin{cases} 1, & i = 1, 2, \\ a_1, & 3 \leq i \leq n-2. \end{cases}$$

Then, straightforward calculations give $\theta_2 = \theta_1 = 1, \theta_3 = a_1 - \kappa^2$, and for $4 \leq i \leq n-2$,

$$\theta_i = a_1 \theta_{i-1} - \kappa^2 a_1 \theta_{i-2}. \tag{4.8}$$

Rewrite (4.8) as follows:

$$\begin{aligned} \theta_i - \zeta_+ \theta_{i-1} &= \zeta_- (\theta_{i-1} - \zeta_+ \theta_{i-2}) = \zeta_-^{i-3} (\theta_3 - \zeta_+ \theta_2), \\ \theta_i - \zeta_- \theta_{i-1} &= \zeta_+ (\theta_{i-1} - \zeta_- \theta_{i-2}) = \zeta_+^{i-3} (\theta_3 - \zeta_- \theta_2), \end{aligned}$$

where $\zeta_+ = \frac{a_1 + \sqrt{a_1^2 - 4\kappa^2 a_1}}{2}$ and $\zeta_- = \frac{a_1 - \sqrt{a_1^2 - 4\kappa^2 a_1}}{2}$, which implies

$$\theta_i = \zeta_+^{i-2} \frac{\theta_3 - \zeta_- \theta_2}{\zeta_+ - \zeta_-} - \zeta_-^{i-2} \frac{\theta_3 - \zeta_+ \theta_2}{\zeta_+ - \zeta_-}. \tag{4.9}$$

Similarly, we can calculate that $\phi_{n-2} = a_1$ and for $i = n-3, \ldots, 3$,

$$\phi_i = a_1 \phi_{i+1} - \kappa^2 a_1 \phi_{i+2}, \tag{4.10}$$

which means

$$\begin{aligned} \phi_3 &= \zeta_+^{n-4} \frac{\phi_{n-2} - \zeta_- \phi_{n-1}}{\zeta_+ - \zeta_-} - \zeta_-^{n-4} \frac{\phi_{n-2} - \zeta_+ \phi_{n-1}}{\zeta_+ - \zeta_-}, \\ \phi_4 &= \zeta_+^{n-5} \frac{\phi_{n-2} - \zeta_- \phi_{n-1}}{\zeta_+ - \zeta_-} - \zeta_-^{n-5} \frac{\phi_{n-2} - \zeta_+ \phi_{n-1}}{\zeta_+ - \zeta_-}, \end{aligned}$$

and $\phi_2 = \phi_3 - \kappa^2 \phi_4$.

Then, we have $(\mathbf{A}^{-1})_{11} = \frac{\phi_2}{\theta_{n-2}}$ and $(\mathbf{A}^{-1})_{12} = \frac{\kappa^3 \phi_3}{\theta_{n-2}}$; (4.7) is equivalent to

$$a_1 = \frac{2\kappa^2 \phi_3 - \kappa^4 \phi_4}{\theta_{n-2}}, \tag{4.11}$$

which can be further simplified as

$$\frac{1}{\zeta_+ - \zeta_-}\left[\left(\zeta_+^{n-2} - \zeta_-^{n-2}\right) - 2\kappa^2\left(\zeta_+^{n-3} - \zeta_-^{n-3}\right) + \kappa^4\left(\zeta_+^{n-4} - \zeta_-^{n-4}\right)\right] = 0. \tag{4.12}$$

Let $\mu_\pm := \frac{s \pm \sqrt{s^2 - s}}{2}$; define a polynomial $p_n(s)$ as follows:

$$p_n(s) := \frac{1}{\mu_+ - \mu_-}\left[16(\mu_+^{n-2} - \mu_-^{n-2}) - 8(\mu_+^{n-3} - \mu_-^{n-3}) + (\mu_+^{n-4} - \mu_-^{n-4})\right].$$

Then, a_1 is a solution of (4.12) if and only if $\frac{a_1}{1+c_+}$ is a root of $p_n(s)$. Straightforward calculations can further give

$$a_i = \begin{cases} \kappa^{-3}a_1 - \kappa^{-1}, & i = 2, \\ \kappa^{i-3} \cdot \frac{\zeta_+^{n-1-i} - \zeta_-^{n-1-i}}{(a_1 - \kappa^2)(\zeta_+^{n-4} - \zeta_-^{n-4})}, & 3 \le i \le n-2. \end{cases} \tag{4.13}$$

If a_1 is the largest root of (4.12), then $\lambda_n := \frac{a_1}{1+c_+}$ is the largest root of $p_n(s)$. By Theorem 3.5 and $\lambda_4 = \frac{1}{2} > \frac{1}{4}$, we can guarantee that $a_i > 0$ for $i = 2, \dots, n-2$ if λ_n is the largest root of $p_n(s)$. Then

$$\begin{aligned} &e_2^{k+1} + (a_2 - \kappa a_3)e_3^{k+1} + \cdots + (a_{n-3} - \kappa a_{n-2})e_{n-2}^{k+1} + a_{n-2}e_{n-1}^{k+1} \\ &\le a_1\left(e_2^k + (a_2 - \kappa a_3)e_3^k + \cdots + (a_{n-3} - \kappa a_{n-2})e_{n-2}^k + a_{n-2}e_{n-1}^k\right), \end{aligned}$$

which means

$$\begin{aligned} \tau_n^- &\le \lim_{k\to\infty} \frac{e_2^{k+1} + (a_2 - \kappa a_3)e_3^{k+1} + \cdots + (a_{n-3} - \kappa a_{n-2})e_{n-2}^{k+1} + a_{n-2}e_{n-1}^{k+1}}{e_2^k + (a_2 - \kappa a_3)e_3^k + \cdots + (a_{n-3} - \kappa a_{n-2})e_{n-2}^k + a_{n-2}e_{n-1}^k} \\ &\le a_1 = \lambda_n(1 + c_+). \end{aligned}$$

Therefore, we complete this proof.

5. Numerical experiments.

In this section, we verify our convergence analyses by implementing the leapfrog algorithm on two Riemannian manifolds: (1) the unit 2-sphere $\mathbb{S}^2$ and (2) the manifold of all 2×2 symmetric positive definite matrices SPD(2). With respect to the standard Euclidean metric, $\mathbb{S}^2$ is a surface of constant positive (+1) sectional curvature. With respect to the affine-invariant metric [21], SPD(2) is a Hadamard manifold, i.e., a manifold with nonpositive sectional curvature. Since the geodesics on these two manifolds can be given in closed form, we can directly compute the following quantity and compare with our theoretical results,

$$r_i^k := \frac{d(y_i^{k+1}, y_i^\infty)}{d(y_i^k, y_i^\infty)} = \frac{e_i^{k+1}}{e_i^k}, \tag{5.1}$$

where $1 \le i \le n-1$ and $k \ge 1$.

5.1. Unit 2-sphere.

Let $\mathbb{S}^2 := \{(z_1, z_2, z_3) | z_1^2 + z_2^2 + z_3^2 = 1\}$ be the unit 2-sphere endowed with the standard Euclidean metric. Then the geodesic joining two nonconjugate points x and y on $\mathbb{S}^2$ is given by

$$\gamma_{x,y}(t) = \frac{\sin((1-t)d(x,y))}{\sin(d(x,y))}x + \frac{\sin(td(x,y))}{\sin(d(x,y))}y, \tag{5.2}$$

where $d(x,y) = \arccos(\langle x, y\rangle)$ is the geodesic distance between x and y.

In the experiment, we set $x_0 = (0, 0, 1)$ and $x_1 = (\frac{1}{2}, \frac{\sqrt{3}}{2}, 0)$. We choose equally distributed points on the line segment joining x_0 and x_1 and then project them onto the sphere as the initial junctions for the leapfrog algorithm. Figure 3 shows the comparison results for $n = 5$ and $n = 7$. We can observe that $\tau_{i,n} = \tau_n^- = \lambda_n$. Moreover, leapfrog gets slower if more junctions are used.

Now we change the initial junctions as follows: initial junctions are chosen as points that equally divide the spherical coordinates, i.e., let $(\cos\alpha \sin\beta, \sin\alpha \sin\beta, \cos\beta)$ be the parameterization of a unit 2-sphere; then the initial junctions are equally distributed in the sense of dividing the parameter space (α, β) equally. From Figure 4, we find there is a (small) gap between the convergence ratio and the maximal root of $p_n(s)$. For $n = 5$, $\tau_{i,5} - \lambda_5 = 0.7235 - 0.6545 = 0.0690$; for $n = 7$, $\tau_{i,7} - \lambda_7 = 0.8537 - 0.8117 = 0.0420$. Therefore, $\tau_{i,n} = \tau_n^- \leq \lambda_n(1 + c_+)$ for some c_+, which is consistent with Theorem 3.1. By comparing Figures 3 and 4, we can observe that different choice of initial junctions will result in different convergence rates.

5.2. Manifold of symmetric positive definite matrices. Let

$$\mathrm{SPD}(2) := \left\{ \begin{bmatrix} a & c \\ c & b \end{bmatrix} | a > 0, ab - c^2 > 0 \right\}$$

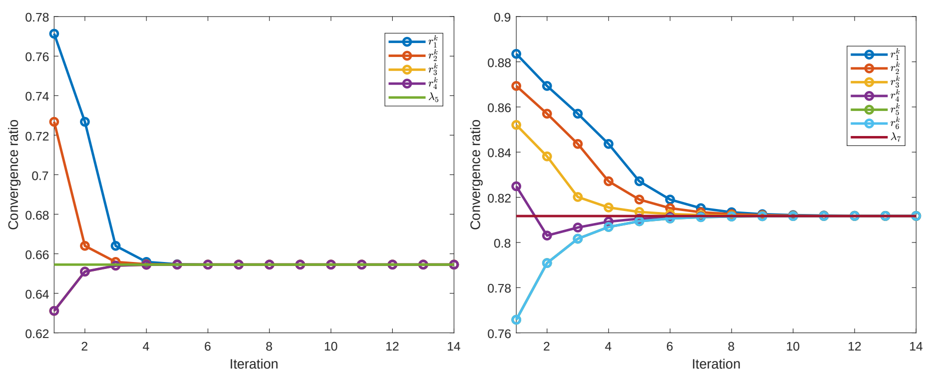

FIG. 3. *Comparison of convergence ratio r_i^k of the leapfrog algorithm on S^2 for $n = 5$ (left) and $n = 7$ (right).*

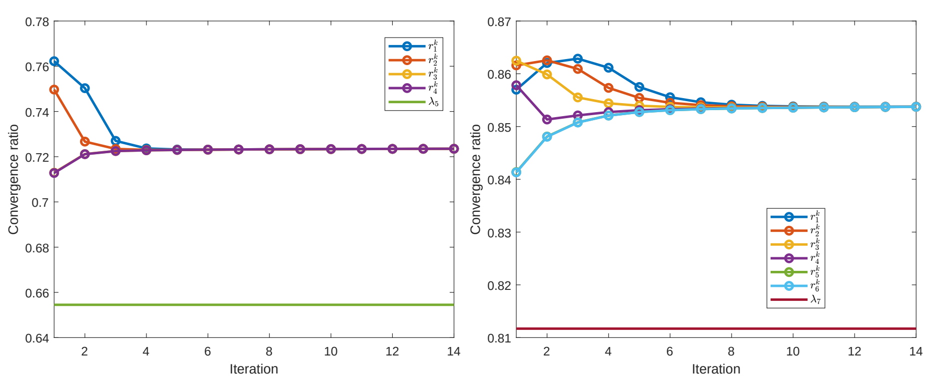

FIG. 4. *Comparison of convergence ratio r_i^k of the leapfrog algorithm on S^2 for $n = 5$ (left) and $n = 7$ (right).*

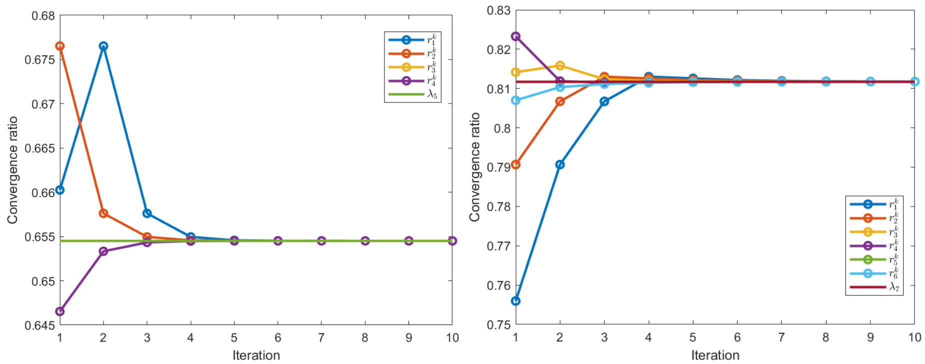

FIG. 5. *Comparison of convergence ratio r_i^k of the leapfrog algorithm on $SPD(2)$ for $n=5$ (left) and $n=7$ (right).*

be the manifold of all 2×2 symmetric positive definite matrices, which is equipped with the following affine-invariant metric:

$$\langle u,v\rangle_x := \langle x^{-1/2}\star u, x^{-1/2}\star v\rangle_{I_2}, \tag{5.3}$$

where $u,v\in T_x\mathrm{SPD}(2)$, $x\in\mathrm{SPD}(2)$, $x^{-1/2}\star u = x^{-1/2}ux^{-1/2}$, $\langle\cdot,\cdot\rangle_{I_2}$ is the Frobenius inner product. Then the geodesic joining two points x and y on SPD(2) is given by

$$\gamma_{x,y}(t) = x\exp(t\log(x^{-1}y)), \tag{5.4}$$

where $\exp(\cdot)$, $\log(\cdot)$ are the matrix exponential and logarithm, respectively. The geodesic distance between x and y is given by

$$d(x,y) = \sqrt{\mathrm{tr}((\log(x^{-1}y))^2)}, \tag{5.5}$$

where $\mathrm{tr}(\cdot)$ is the trace of a matrix. The differential geometry of SPD and its applications can be found in [21, 20, 25].

In the experiment, we set x_0 as the 2×2 identity matrix I_2 and $x_1 = [\begin{smallmatrix}4 & 2\\ 2 & 3\end{smallmatrix}]$. The initial junctions are chosen as $y_i = x_0 + \frac{i}{n}(x_1 - x_0)$ with $i=1,2,\ldots,n-1$. Figure 5 shows the comparison results for $n=5$ and $n=7$, from which we can observe that $\tau_n^+ = \tau_n^- = \lambda_n$.

6. Conclusions. Geodesics are of fundamental interest in theoretical studies and applications. Noakes [15] proposed the so-called *leapfrog algorithm* to find geodesics joining two given points on a complete path-connected Riemannian manifold and proved the sequence of piecewise geodesics $\{\gamma^k\}$ generated by this algorithm converges to the desired geodesic. However, the convergence rate is not known in the literature, to the authors' best knowledge. In the present paper, we firstly analyze the relationship between e_{i-1}^{k+1}, e_i^{k+1}, and e_{i+1}^k by taking advantage of the estimation of the geodesic distance. Then, by considering the relationship between a linear combination of e_i^{k+1} and that of e_i^k, we find that the fastest convergent rate of junctions is upper bounded by $\lambda_n(1+c_+)$, where λ_n is the largest root of the polynomial $p_n(s)$ (see (3.1)) and $c_+\in[0,1)$ is some small constant. Further, λ_n increases as n increases, which somehow implies leapfrog is slower if more junctions are used. Finally, we verify our theoretical analyses on the unit 2-sphere $\mathbb{S}^2$ and the manifold SPD(2) of 2×2 symmetric positive definite matrices.

Note that our whole analyses heavily depend on Lemmas 2.2 and 2.3, which assumes that junctions are reasonably nearby. However, it is hard to give the closeness measure of junctions in practice. Beside, if we can present better estimations for the constant c_+, it is possible to refine the results in this paper, which could be our future work. Other future research directions may include considering convergence rate of the leapfrog algorithm for control problems and other optimization problems.

Appendix A. Proof of Lemma 2.2. Choosing normal coordinates at x, we get $p=\frac{1}{2}y$ and $q=\frac{1}{2}z$. By Lemma 2.1, we have

$$d^2(p,q)-\frac{1}{4}d^2(y,z)=\frac{1}{16}\langle R(z,y)y,z\rangle+\mathcal{O}(\delta^4),$$

which indicates

$$\begin{aligned}\frac{d^2(p,q)}{d^2(y,z)}-\frac{1}{4}&=\frac{1}{16}\frac{\langle R(z,y)y,z\rangle}{d^2(y,z)}+\mathcal{O}(\delta^2)\\&=\frac{1}{16}\|y\|^2\left\langle R\left(\frac{z-y}{\|z-y\|},\frac{y}{\|y\|}\right)\frac{y}{\|y\|},\frac{z-y}{\|z-y\|}\right\rangle+\mathcal{O}(\delta^2)\\&=\frac{1}{16}\|y\|^2K(z-y,y)\left(1-\left\langle\frac{z-y}{\|z-y\|},\frac{y}{\|y\|}\right\rangle^2\right)+\mathcal{O}(\delta^2)\\&\le\frac{1}{16}\|y\|^2K(z-y,y)+\mathcal{O}(\delta^2),\end{aligned}$$

where K is the bounded sectional curvature. Since $\|y\|$ is sufficiently small, there exist sufficiently small constants $c_-,c_+\in[0,1)$ such that

$$-\frac{1}{4}c_-\le\frac{d^2(p,q)}{d^2(y,z)}-\frac{1}{4}\le\frac{1}{4}c_+,$$

which proves (2.2).

Now we prove the case where M has nonpositive sectional curvature (the other one is similar). By Toponogov's theorem [7], we have

$$\begin{aligned}d^2(z,p)&\le\frac{1}{2}d^2(z,x)+\frac{1}{2}d^2(z,y)-\frac{1}{4}d^2(x,y),\\d^2(y,q)&\le\frac{1}{2}d^2(y,z)+\frac{1}{2}d^2(y,x)-\frac{1}{4}d^2(x,z),\\d^2(p,q)&\le\frac{1}{2}d^2(p,x)+\frac{1}{2}d^2(p,z)-\frac{1}{4}d^2(x,z),\\d^2(q,p)&\le\frac{1}{2}d^2(q,x)+\frac{1}{2}d^2(q,y)-\frac{1}{4}d^2(x,y),\end{aligned}$$

from which we eliminate $d^2(z,p)$ and $d^2(y,q)$; then

$$\begin{aligned}2d^2(p,q)&\le\frac{1}{2}d^2(p,x)+\frac{1}{2}d^2(q,x)+\frac{1}{2}d^2(y,z)-\frac{1}{8}d^2(x,y)-\frac{1}{8}d^2(x,z)\\&=\frac{1}{2}d^2(y,z),\end{aligned}$$

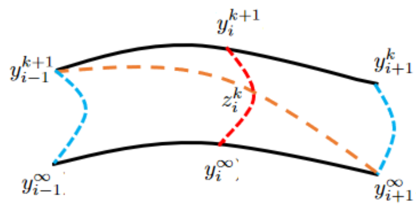

FIG. 6. *An illustration of three consecutive junctions.*

where we have used $d(p,x) = \frac{1}{2}d(x,y)$ and $d(q,x) = \frac{1}{2}d(x,z)$. Therefore, we get the inequality $d(p,q) \leq \frac{1}{2}d(y,z)$.

Appendix B. Proof of Lemma 2.3. When $i=1$ or $n-1$, this lemma follows from Lemma 2.2 directly. Now we consider $1<i<n-1$. Let z_i^k be the midpoint of the geodesic joining y_{i-1}^{k+1} and y_{i+1}^{∞} (see Figure 6); then by the triangle inequality of the distance function,

$$e_i^{k+1} \leq d\left(y_i^{k+1}, z_i^k\right) + d\left(z_i^k, y_i^{\infty}\right) \leq \frac{1}{2}\sqrt{1+c_+}\left(e_{i-1}^{k+1} + e_{i+1}^{k}\right), \tag{B.1}$$

where we have used Lemma 2.2 twice in the last inequality.

Appendix C. Proof of Theorem 2.4. By Lemma 2.3, we have

$$\begin{cases} e_1^{k+1} \leq \kappa e_2^k, \\ e_2^{k+1} \leq \kappa\left(e_1^{k+1} + e_3^k\right), \\ e_3^{k+1} \leq \kappa\left(e_2^{k+1} + e_4^k\right), \\ \cdots \\ e_{n-2}^{k+1} \leq \kappa\left(e_{n-3}^{k+1} + e_{n-1}^k\right), \\ e_{n-1}^{k+1} \leq \kappa e_{n-2}^{k+1}, \end{cases}$$

$$\Longrightarrow \begin{cases} e_2^{k+1} \leq \kappa^2 e_2^k + \kappa e_3^k, \\ e_3^{k+1} \leq \kappa^3 e_2^k + \kappa^2 e_3^k + \kappa e_4^k, \\ \cdots \\ e_{n-2}^{k+1} \leq \kappa^{n-2} e_2^k + \kappa^{n-3} e_3^k \cdots + \kappa^2 e_{n-2}^k + \kappa e_{n-1}^k. \end{cases}$$

Then we get

$$\max_{2\leq i\leq n-1} e_i^{k+1} \leq \left(\kappa^{n-2} + \kappa^{n-3} + \cdots + \kappa^2 + \kappa\right) \max_{2\leq i\leq n-1} e_i^k = \frac{\kappa(1-\kappa^{n-2})}{1-\kappa} \max_{2\leq i\leq n-1} e_i^k,$$

which indicates the limitation of $\frac{\|v^{k+1}\|_\infty}{\|v^k\|_\infty}$ is upper bounded by $\frac{\kappa(1-\kappa^{n-2})}{1-\kappa}$.

Appendix D. Roots of the polynomial $q_n(s)$. The main purpose of this section is to prove that the polynomial $q_n(s)$ has $\lceil \frac{n}{2} \rceil - 1$ distinct real roots.

LEMMA D.1. *The polynomial $q_n(s)$ is given as follows:*

$$
\begin{aligned}
q_{2k}(s) &= \alpha_+^{k-2} q_4(s) + (q_6(s) - \alpha_+ q_4(s)) \frac{\alpha_+^{k-2} - \alpha_-^{k-2}}{\alpha_+ - \alpha_-} \\
&= \alpha_-^{k-2} q_4(s) + (q_6(s) - \alpha_- q_4(s)) \frac{\alpha_+^{k-2} - \alpha_-^{k-2}}{\alpha_+ - \alpha_-}, \\
q_{2k+1}(s) &= \alpha_+^{k-2} q_5(s) + (q_7(s) - \alpha_+ q_5(s)) \frac{\alpha_+^{k-2} - \alpha_-^{k-2}}{\alpha_+ - \alpha_-} \\
&= \alpha_-^{k-2} q_5(s) + (q_7(s) - \alpha_- q_5(s)) \frac{\alpha_+^{k-2} - \alpha_-^{k-2}}{\alpha_+ - \alpha_-},
\end{aligned} \tag{D.1}
$$

where $\alpha_\pm = \mu_\pm - \frac{1}{4}$, $k \geq 2$.

Proof. We only prove the first expression, and the others are similar. By the recurrence relationship (3.6), we have

$$
q_{2k} = \left(s - \frac{1}{2}\right) q_{2k-2} - \frac{1}{16} q_{2k-4},
$$

which implies

$$
q_{2k} - \alpha_+ q_{2k-2} = \alpha_- (q_{2k-2} - \alpha_+ q_{2k-4}) = \alpha_-^{k-3} (q_6 - \alpha_+ q_4).
$$

By induction, we get

$$
\begin{aligned}
q_{2k} &= \alpha_+^{k-2} q_4 + (q_6 - \alpha_+ q_4) \left(\alpha_-^{k-3} + \cdots + \alpha_+^i \alpha_-^{k-3-i} + \cdots + \alpha_+^{k-3}\right) \\
&= \alpha_+^{k-2} q_4 + (q_6 - \alpha_+ q_4) \frac{\alpha_+^{k-2} - \alpha_-^{k-2}}{\alpha_+ - \alpha_-}.
\end{aligned}
$$

∎

LEMMA D.2. *For $k \geq 2$,*

$$
\begin{aligned}
q_{2k}(1-s) &= (-1)^{k-1} q_{2k}(s), \\
q_{2k+1}(1-s) &= (-1)^{k-2} q_{2k+1}(s) + \frac{1}{2} (-1)^{k-1} q_{2k}(s),
\end{aligned}
$$

which means all roots of q_{2k} are symmetric with respect to $s = \frac{1}{2}$ and all roots of q_{2k} are not symmetric with respect to $s = \frac{1}{2}$.

Proof. Straightforward calculations show that

$$
\begin{aligned}
q_4(1-s) &= -16s + 8 = -q_4(s), \\
q_5(1-s) &= 16s^2 - 20s + 5 = q_5(s) - \frac{1}{2} q_4(s), \\
q_6(1-s) &= 16s^2 - 16s + 3 = q_6(s), \\
q_7(1-s) &= -16s^3 + 28s^2 - 14s + \frac{7}{4} = -q_7(s) + \frac{1}{2} q_6(s).
\end{aligned}
$$

Then, by Lemma D.1,

$$\begin{aligned} q_{2k}(1-s) &= (-1)^{k-2}\alpha_-^{k-2}(-q_4(s)) + (q_6(s)-\alpha_- q_4(s))\frac{(-1)^{k-2}(\alpha_+^{k-2}-\alpha_-^{k-2})}{-(\alpha_+-\alpha_-)} \\ &= (-1)^{k-1}q_{2k}(s), \\ q_{2k+1}(1-s) &= (-1)^{k-2}\alpha_-^{k-2}\left(q_5(s)-\frac{1}{2}q_4(s)\right) \\ &\quad + \left(-q_7(s)+\frac{1}{2}q_6(s)+\alpha_-\left(q_5(s)-\frac{1}{2}q_4(s)\right)\right)\frac{(-1)^{k-2}(\alpha_+^{k-2}-\alpha_-^{k-2})}{-(\alpha_+-\alpha_-)} \\ &= (-1)^{k-2}q_{2k+1}(s)+\frac{1}{2}(-1)^{k-1}q_{2k}(s). \qquad \square \end{aligned}$$

Note that any q_n and q_{n+1} or q_n and q_{n+2} do not share same roots; otherwise, all polynomials share same roots by the recurrence relationship (3.6), which contradicts with the fact that q_4 and q_5 do not share same roots.

Lemma D.3. *Suppose q_n has $\lceil \frac{n}{2} \rceil - 1$ distinct real roots on $(0,1)$ when $n \le n_0$ for some integer n_0. Let*

$$\begin{aligned} &0<\delta_1<\cdots<\delta_k<1, \\ &0<\theta_1<\cdots<\theta_k<1, \\ &0<\eta_1<\cdots<\eta_{k-1}<1 \end{aligned}$$

be roots of q_{2k+2}, q_{2k+1}, and q_{2k}, respectively. Then, these roots satisfy

$$\begin{aligned} &0<\theta_1<\eta_1<\cdots<\theta_i<\eta_i<\theta_{i+1}<\cdots<\eta_{k-1}<\theta_k<1, \\ &0<\theta_1<\delta_1<\cdots<\theta_i<\delta_i<\theta_{i+1}<\cdots<\theta_k<\delta_k<1. \end{aligned} \tag{D.2}$$

Proof. By checking roots of q_4, q_5, and q_6, we can easily find

$$\begin{aligned} &0<\theta_1=\frac{3-\sqrt{5}}{8}<\eta_1=\frac{1}{2}<\theta_2=\frac{3+\sqrt{5}}{8}<1, \\ &0<\theta_1=\frac{3-\sqrt{5}}{8}<\delta_1=\frac{1}{4}<\theta_2=\frac{3+\sqrt{5}}{8}<\delta_2=\frac{3}{4}<1. \end{aligned}$$

Suppose (D.2) is true for integers until k. Now we consider the case of $k+1$. Let

$$\begin{aligned} &0<\delta_1^*<\cdots<\delta_{k+1}^*<1, \\ &0<\theta_1^*<\cdots<\theta_{k+1}^*<1 \end{aligned}$$

be roots of q_{2k+4} and q_{2k+3}, respectively.

By the recurrence relationship $q_{2k+3}=sq_{2k+2}-\frac{1}{4}q_{2k+1}$, we have

$$\begin{aligned} &\theta_k<\delta_k<1 \implies q_{2k+3}(\delta_k)=-\frac{1}{4}q_{2k+1}(\delta_k)<0, \\ &\theta_{k-1}<\delta_{k-1}<\theta_l \implies q_{2k+3}(\delta_{k-1})=-\frac{1}{4}q_{2k+1}(\delta_{k-1})>0. \end{aligned}$$

Then, δ_k belongs to one of the following intervals:

$$(\theta_k^*,\theta_{k+1}^*),\ (\theta_{k-2}^*,\theta_{k-1}^*),\ (\theta_{k-4}^*,\theta_{k-3}^*),\ \ldots.$$

Suppose $\delta_k \in (\theta^*_{k-2u}, \theta^*_{k-2u+1})$ for some $0 \le u \le \lfloor \frac{k}{2} \rfloor$; then δ_{k-1} belongs to one of the following intervals:

$$(\theta^*_{k-2u-1}, \theta^*_{k-2u}),\ (\theta^*_{k-2u-3}, \theta^*_{k-2u-2}),\ (\theta^*_{k-2u-5}, \theta^*_{k-2u-4}),\ \ldots.$$

By repeating this argument and the number of distinct real roots, we have $\theta^*_{k-1} < \delta_{k-1} < \theta^*_k < \delta_k < \theta^*_{k+1}$. By induction, we can verify

$$0 < \theta^*_1 < \delta_1 < \cdots < \theta^*_i < \delta_i < \theta^*_{i+1} < \cdots < \delta_k < \theta^*_{k+1} < 1.$$

Similarly, by $q_{2k+4} = q_{2k+3} - \frac{1}{4} q_{2k+2}$, we have

$$\delta_k < \theta^*_{k+1} < 1 \implies q_{2k+4}(\theta^*_{k+1}) = -\frac{1}{4} q_{2k+2}(\theta^*_{k+1}) < 0,$$
$$\delta_{k-1} < \theta^*_k < \delta_k \implies q_{2k+4}(\theta^*_k) = -\frac{1}{4} q_{2k+2}(\theta^*_k) > 0.$$

Then, θ^*_{k+1} belongs to one of the following intervals:

$$(\delta^*_k, \delta^*_{k+1}),\ (\delta^*_{k-2}, \delta^*_{k-1}),\ (\delta^*_{k-4}, \delta^*_{k-3}),\ \ldots.$$

Suppose $\theta^*_{k+1} \in (\delta^*_{k-2u}, \delta^*_{k-2u+1})$ for some $0 \le u \le \lfloor \frac{k}{2} \rfloor$; then θ^*_k belongs to one of the following intervals:

$$(\delta^*_{k-2u-1}, \delta^*_{k-2u}),\ (\delta^*_{k-2u-3}, \delta^*_{k-2u-2}),\ (\delta^*_{k-2u-5}, \delta^*_{k-2u-4}),\ \ldots.$$

By repeating this argument and the number of distinct real roots, we have $\delta^*_{k-1} < \theta^*_k < \delta^*_k < \theta^*_{k+1} < \delta^*_{k+1}$. By induction, we can verify

$$0 < \theta^*_1 < \delta^*_1 < \cdots < \theta^*_i < \delta^*_i < \theta^*_{i+1} < \cdots < \theta^*_{k+1} < \delta^*_{k+1} < 1. \qquad \square$$

LEMMA D.4. *For $n \ge 9$, $4 \le i \le n-5$, q_n satisfies*

$$q_n = \frac{1}{16}\left(\left(s^{\frac{1-(-1)^n}{2}}\right)^{\frac{1-(-1)^i}{2}} q_{i+1} q_{n-i} - \frac{1}{4}\left(s^{\frac{1-(-1)^n}{2}}\right)^{\frac{1+(-1)^i}{2}} q_i q_{n-1-i}\right).$$

Proof. By induction on the recurrence relationship (3.6), we have

$$q_n = s^{\frac{1-(-1)^n}{2}} q_{n-1} - \frac{1}{4} q_{n-2},$$
$$q_{n-1} = s^{\frac{1-(-1)^{n-1}}{2}} q_{n-2} - \frac{1}{4} q_{n-3},$$
$$\cdots$$
$$q_{n-i} = s^{\frac{1-(-1)^{n-i}}{2}} q_{n-1-i} - \frac{1}{4} q_{n-2-i}.$$

Multiplying the first equation by $c_0 = 1$, the second equation by $c_1 = s^{\frac{1-(-1)^n}{2}}$, and the $(i+1)$th equation by c_i, where $c_i = s^{\frac{1-(-1)^{n+1-i}}{2}} c_{i-1} - \frac{1}{4} c_{i-2}$, and summing them together gives

$$q_n = \left(s^{\frac{1-(-1)^{n-i}}{2}} c_i - \frac{1}{4} c_{i-1}\right) q_{n-1-i} - \frac{1}{4} c_i q_{n-2-i} = c_i q_{n-i} - \frac{1}{4} c_{i-1} q_{n-1-i}.$$

By induction, we get $c_i = \frac{1}{16}(s^{\frac{1-(-1)^n}{2}})^{\frac{1-(-1)^i}{2}} q_{i+1}$, which completes this proof. $\square$

THEOREM D.5. *The polynomial* q_n $(n \geq 4)$ *has* $\lceil \frac{n}{2} \rceil - 1$ *distinct real roots on* $(0,1)$.

Proof. By straightforward calculations, we can verify this claim is true for $n = 4, 5, 6, 7$. Suppose it holds until $n-1$; now we intend to verify the case of n.

(1) If n is odd, i.e., $n = 2m+1$ for some m, then Lemma D.4 implies

$$q_n = \frac{1}{16}\left(s^{\frac{1-(-1)^m}{2}} q_{m+1}^2 - \frac{1}{4} s^{\frac{1+(-1)^m}{2}} q_m^2 \right).$$

(i) If m is odd, i.e., $m = 2k+1$ for some k, then

$$q_n = \frac{1}{16}\left(s q_{2k+2}^2 - \frac{1}{4} q_{2k+1}^2 \right).$$

By assumption, both q_{2k+2} and q_{2k+1} have k distinct real roots on $(0,1)$. Let

$$0 < \delta_1 < \cdots < \delta_k < 1,$$
$$0 < \theta_1 < \cdots < \theta_k < 1$$

be roots of q_{2k+2} and q_{2k+1}, respectively; then Lemma D.3 implies

$$0 < \theta_1 < \delta_1 < \cdots < \theta_i < \delta_i < \theta_{i+1} < \cdots < \theta_k < \delta_k < 1.$$

Since

$$q_n(0) < 0, \quad q_n(\theta_1) = \frac{1}{16}\theta_1 q_{2k+2}^2(\theta_1) > 0, \quad q_n(\delta_1) = -\frac{1}{64} q_{2k+1}^2(\delta_1) < 0, \quad \ldots,$$
$$q_n(\theta_i) = \frac{1}{16}\theta_i q_{2k+2}^2(\theta_i) > 0, \quad q_n(\delta_i) = -\frac{1}{64} q_{2k+1}^2(\delta_i) < 0, \quad \ldots, \quad q_n(1) > 0.$$

By the mean value theorem, q_n has $2k+1 = m = \lceil \frac{n}{2} \rceil - 1$ distinct real roots on $(0,1)$.

(ii) If m is even, i.e., $m = 2k$ for some k, then

$$q_n = \frac{1}{16}\left(q_{2k+1}^2 - \frac{1}{4} s q_{2k}^2 \right).$$

By assumption, q_{2k+1} and q_{2k} have k and $k-1$ distinct real roots on $(0,1)$, respectively. Let

$$0 < \theta_1 < \cdots < \theta_k < 1,$$
$$0 < \eta_1 < \cdots < \eta_{k-1} < 1$$

be roots of q_{2k+1} and q_{2k}, respectively; then Lemma D.3 implies

$$0 < \theta_1 < \eta_1 < \cdots < \theta_i < \eta_i < \theta_{i+1} < \cdots < \eta_{k-1} < \theta_k < 1.$$

Since

$$q_n(0) > 0, \quad q_n(\theta_1) = -\frac{1}{64}\theta_1 q_{2k}^2(\theta_1) < 0, \quad q_n(\eta_1) = \frac{1}{16} q_{2k+1}^2(\eta_1) > 0, \quad \ldots,$$
$$q_n(\theta_i) = -\frac{1}{64}\theta_i q_{2k}^2(\theta_i) < 0, \quad q_n(\eta_i) = \frac{1}{16} q_{2k+1}^2(\eta_i) > 0, \quad \ldots, \quad q_n(1) > 0.$$

By the mean value theorem, q_n has $2k = m = \lceil \frac{n}{2} \rceil - 1$ distinct real roots on $(0,1)$.

(2) If n is even, i.e., $n = 2m$ for some m, then Lemma D.4 implies

$$q_n = \frac{1}{16} q_m \left(q_{m+1} - \frac{1}{4} q_{m-1} \right).$$

(i) If m is odd, i.e., $m = 2k+1$ for some k, then by assumption and Lemma D.2, q_m has k distinct real roots on $(0,1)$, which are not symmetric with respect to $s = \frac{1}{2}$ (note $q_{2k+1}(\frac{1}{2}) \neq 0$). Since all roots of q_n are symmetric with respect to $s = \frac{1}{2}$, therefore, q_n has $2k$ distinct real roots on $(0,1)$.

(ii) If m is even, i.e., $m = 2k$ for some k, then

$$q_n = \frac{1}{16} q_{2k} \left(2q_{2k+1} - s q_{2k}\right).$$

By assumption, q_{2k+1} and q_{2k} have k and $k-1$ distinct real roots on $(0,1)$, respectively. Let

$$0 < \theta_1 < \cdots < \theta_k < 1,$$
$$0 < \eta_1 < \cdots < \eta_{k-1} < 1$$

be roots of q_{2k+1} and q_{2k}, respectively; then Lemma D.3 implies

$$0 < \theta_1 < \eta_1 < \cdots < \theta_i < \eta_i < \theta_{i+1} < \cdots < \eta_{k-1} < \theta_k < 1.$$

Define $Q := 2q_{2k+1} - s q_{2k}$. We have

$$Q(0) = 2q_{2k+1}(0) = 2\left(-\frac{1}{4}\right)^{k-2}, \quad Q(\theta_1) = -\theta_1 q_{2k}(\theta_1), \quad Q(\eta_1) = 2q_{2k+1}(\eta_1), \quad \ldots,$$
$$Q(\theta_i) = -\theta_i q_{2k}(\theta_i), \quad Q(\eta_i) = 2q_{2k+1}(\eta_i), \ldots,$$
$$Q(1) = 2q_{2k+1}(1) - q_{2k}(1) = 2(-1)^{k-2} q_{2k+1}(0) = 2^{5-2k} > 0.$$

If k is odd, then

$$Q(0) < 0, Q(\theta_1) < 0, Q(\eta_1) > 0, Q(\theta_2) > 0, Q(\eta_2) < 0, Q(\theta_3) < 0, Q(\eta_3) > 0, \ldots.$$

If k is even, then

$$Q(0) > 0, Q(\theta_1) > 0, Q(\eta_1) < 0, Q(\theta_2) < 0, Q(\eta_2) > 0, Q(\theta_3) > 0, Q(\eta_3) < 0, \ldots.$$

By the mean value theorem, Q has $k-1$ distinct real roots on $(0,1)$. Note that Q and q_{2k} do not share the same roots. Therefore, q_n has $k + k - 1 = 2k - 1 = m - 1 = \lceil \frac{n}{2} \rceil - 1$ distinct real roots on $(0,1)$. ∎

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REFERENCES

[1] D. Bryner, *Endpoint geodesics on the Stiefel manifold embedded in Euclidean space*, SIAM J. Matrix Anal. Appl., 38 (2017), pp. 1139–1159, https://doi.org/10.1137/16M1103099.

[2] J. Cheeger and D. G. Ebin, *Comparison Theorems in Riemannian Geometry*, North-Holland, Amsterdam, 1975.

[3] P. Chen and S. M. N. Islam, *Optimal control models in finance*, in Optimal Control Models in Finance, Appl. Optim. 95, P. Pardalos and D. W. Hearn, eds., Springer, Boston, 2005, pp. 1–20, https://doi.org/10.1007/0-387-23570-1_1.

[4] P. T. Fletcher, C. Lu, and S. Joshi, *Statistics of shape via principal geodesic analysis on Lie groups*, in Proceedings of the 2003 IEEE Computer Society Conference on Computer Vision and Pattern Recognition, IEEE, Madison, WI, 2003, p. I.

[5] P. T. Fletcher, C. Lu, S. M. Pizer, and S. Joshi, *Principal geodesic analysis for the study of nonlinear statistics of shape*, IEEE Trans. Med. Imaging, 23 (2004), pp. 995–1005, https://doi.org/10.1109/TMI.2004.831793.

[6] P. T. Fletcher, *Geodesic regression on Riemannian manifolds*, in Proceedings of the Third International Workshop on Mathematical Foundations of Computational Anatomy: Geometrical and Statistical Methods for Modelling Biological Shape Variability, MFCA, Toronto, 2011, pp. 75–86.

[7] H. Karcher, *Riemannian Comparison Constructions*, SFB 256, Vol. 5, Universität Bonn, Bonn, Germany, 1987.

[8] C. Y. Kaya and J. L. Noakes, *The leap-frog algorithm and optimal control: Theoretical aspects*, in Proceedings of the International Conference on Optimization: Techniques and Applications, ICOTA, Perth, Australia, 1998.

[9] C. Y. Kaya and J. L. Noakes, *Leapfrog for optimal control*, SIAM J. Numer. Anal., 46 (2008), pp. 2795–2817, https://doi.org/10.1137/060675034.

[10] R. Kozera and L. Noakes, *Non-generic case of leap-frog for optimal knots selection in fitting reduced data*, in Proceedings of the International Conference on Computational Science, 2022, pp. 341–354, https://doi.org/10.1007/978-3-031-08757-8_29.

[11] R. Kozera, L. Noakes, and A. Wiliński, *Generic case of leap-frog algorithm for optimal knots selection in fitting reduced data*, in Proceedings of the International Conference on Computational Science, 2021, pp. 337–350, https://doi.org/10.1007/978-3-030-77970-2_26.

[12] K. A. Krakowski, *Geometrical Methods of Inference*, Ph.D. thesis, University of Western Australia, Crawley, Australia, 2002.

[13] B. Matebese, D. Withey, and M. K. Banda, *Application of the leapfrog method to robot path planning*, in Proceedings of the 2014 IEEE International Conference on Information and Automation (ICIA), IEEE, 2014, Hailar, China, pp. 710–715, https://doi.org/10.1109/ICInfA.2014.6932744.

[14] B. Matebese, D. Withey, and M. K. Banda, *Initialization of the leapfrog algorithm for mobile robot path planning*, in Proceedings of the 2016 Pattern Recognition Association of South Africa and Robotics and Mechatronics International Conference (PRASA-RobMech), IEEE, 2016, Stellenbosch, South Africa, pp. 1–6, https://doi.org/10.1109/RoboMech.2016.7813161.

[15] L. Noakes, *A global algorithm for geodesics*, J. Aust. Math. Soc., 65 (1998), pp. 37–50, https://doi.org/10.1017/S1446788700039380.

[16] L. Noakes and R. Kozera, 2D *leapfrog algorithm for optimal surface reconstruction*, in Vision Geometry VIII, Vol. 3811, L. J. Latecki, R. A. Melter, D. M. Mount, and A. Y. Wu, eds., SPIE, 1999, Denver, CO, pp. 317–328, https://doi.org/10.1117/12.364108.

[17] L. Noakes and R. Kozera, *Nonlinearities and noise reduction in* 3*-source photometric stereo*, J. Math. Imaging Vision, 18 (2003), pp. 119–127, https://doi.org/10.1023/A:1022104332058.

[18] L. Noakes and E. Zhang, *Finding geodesics joining given points*, Adv. Comput. Math., 48 (2022), pp. 1–27, https://doi.org/10.1007/s10444-022-09966-y.

[19] L. Noakes and E. Zhang, *Finding extremals of Lagrangian actions*, Commun. Nonlinear Sci. Numer. Simul., 116 (2023), 106826, https://doi.org/10.1016/j.cnsns.2022.106826.

[20] X. Pennec, *Statistical Computing on Manifolds for Computational Anatomy*, Ph.D. thesis, Université Nice Sophia Antipolis, Nice, France, 2006.

[21] X. Pennec, P. Fillard, and N. Ayache, *A Riemannian framework for tensor computing*, Int. J. Comput. Vis., 66 (2006), pp. 41–66, https://doi.org/10.1007/s11263-005-3222-z.

[22] M. Sutti and B. Vandereycken, *The Leapfrog Algorithm as Nonlinear Gauss-Seidel*, arXiv preprint, arXiv:2010.14137, 2020.

[23] P. Thomas Fletcher, *Geodesic regression and the theory of least squares on Riemannian manifolds*, Int. J. Comput. Vis., 105 (2013), pp. 171–185, https://doi.org/10.1007/s11263-012-0591-y.

[24] R. A. Usmani, *Inversion of Jacobi's tridiagonal matrix*, Comput. Math. Appl., 27 (1994), pp. 59–66, https://doi.org/10.1016/0898-1221(94)90066-3.

[25] E. Zhang and L. Noakes, *Riemannian cubics and elastica in the manifold SPD(n) of all* $n \times n$ *symmetric positive-definite matrices*, J. Geom. Mech., 11 (2019), https://doi.org/10.3934/jgm.2019015.

[26] R. Zimmermann, *A matrix-algebraic algorithm for the Riemannian logarithm on the Stiefel manifold under the canonical metric*, SIAM J. Matrix Anal. Appl., 38 (2017), pp. 322–342, https://doi.org/10.1137/16M1074485.

[27] R. Zimmermann and K. Hüper, *Computing the Riemannian logarithm on the Stiefel manifold: Metrics, methods, and performance*, SIAM J. Matrix Anal. Appl., 43 (2022), pp. 953–980, https://doi.org/10.1137/21M1425426.