Non-Generic Case of Leap-Frog for Optimal Knots Selection in Fitting Reduced Data

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Abstract. The problem of fitting multidimensional reduced data is analyzed here . The missing interpolation knots $\mathcal{T}$ are substituted by $\hat{\mathcal{T}}$ which minimize a non-linear multivariate function $\mathcal{J}_0$. One of numerical schemes designed to compute such optimal knots relies on iterative scheme called *Leap-Frog Algorithm*. The latter is based on merging the respective generic and non-generic univariate overlapping optimizations of $\mathcal{J}_0^{(k,i)}$. The discussion to follow establishes the sufficient conditions enforcing unimodality of the non-generic case of $\mathcal{J}_0^{(k,i)}$ (for special data set-up and its perturbation). Illustrative example supplements the analysis in question. This work complements already existing analysis on generic case of *Leap-Frog Algorithm*.

Keywords: Data fitting · Optimization · Curve modelling

1 Introduction

Assume that n interpolation points $\mathcal{M}_n = \{x_i\}_{i=0}^n$ in arbitrary Euclidean space $\mathbb{E}^m$ are given with the associated knots $\mathcal{T} = \{t_i\}_{i=0}^n$ unavailable. The analyzed here class of fitting curves $\mathcal{I}$ forms piecewise C^2 functions $\gamma : [0, T] \to \mathbb{E}^m$ satisfying $\gamma(t_i) = q_i$ and $\ddot{\gamma}(t_0) = \ddot{\gamma}(T) = \mathbf{0}$. It is also assumed that $\gamma \in \mathcal{I}$ is at least of class C^1 over $\mathcal{T}_{int} = \{t_i\}_{i=1}^{n-1}$ and extends to $C^2([t_i, t_{i+1}])$. *The unknown internal knots $\mathcal{T}_{int}$ are called admissible* if $t_i < t_{i+1}$, for $i = 0, 1, \ldots, n-1$ (here $t_0 = 0$ and $t_n = T$). Different choices of $\mathcal{T}_{int}$ permits *to control and model* the trajectory of γ. A possible criterion (measuring the "average acceleration" of γ) for a given choice of fixed knots $\mathcal{T}$ is to minimize

$$\mathcal{J}_T(\gamma) = \sum_{i=0}^{n-1} \int_{t_i}^{t_{i+1}} \|\ddot{\gamma}(t)\|^2 dt \, , \tag{1}$$

(over $\mathcal{I}$) which yields a unique optimal curve $\gamma_{opt} \in \mathcal{I}$ being *a natural cubic spline* γ_{NS} - see [1,9]. Thus, varying $\mathcal{T}_{int}$ reformulates (1) into searching for an optimal natural spline γ_{NS} with $\mathcal{T}_{int}$ treated as free variables. As shown in [3] the latter reformulates into optimizing a highly non-linear function J_0 in $n-1$ variables $\mathcal{T}_{int}$ subject to $t_i < t_{i+1}$. Due to the complicated nature of J_0 most of numerical schemes used to optimize J_0 face numerical difficulties (see e.g. [3]). Equally, studying the character of critical points of J_0 forms a non-trivial task. A possible remedy is to apply *a Leap-Frog Algorithm* (see [2,3]) designed to optimize J_0 upon merging the iterative sequence of univariate overlapping optimizations of $J_0^{(k,i)}$ preserving $t_i < t_{i+1}$. Recent work [5] deals with *the generic case* of *a Leap-Frog* recomputing iteratively the knots $\{t_2, t_3, \ldots, t_{n-2}\}$.

This paper discusses[1] *a non-generic* case of *Leap-Frog* covering the recursive readjustment of knots t_1 and t_{n-1}. The latter establishes sufficient conditions for *unimodality* of $J_0^{(k,1)}$ and $J_0^{(k,n-1)}$. First a special data case (18) is considered (see Sect. 4) which in turn is subsequently extended to its perturbed version (22) preserving in practice the unimodality (once it occurs for (18)) for substantially large perturbations (see Proposition 1 and Example 1 in Sect. 5).

Numerical performance of *Leap-Frog* and comparison tests with other optimization schemes are presented in [2,3,7]. Some applications of *Leap-Frog* optimization scheme in modelling and simulation are covered in [10–12].

2   Preliminaries

A cubic spline interpolant (see [1]) $\gamma_{\mathcal{T}}^{C_i} = \gamma_{\mathcal{T}}^C|_{[t_i, t_{i+1}]}$, for a given admissible knots $\mathcal{T} = (t_0, t_1, \ldots, t_{n-1}, t_n)$ defined as $\gamma_{\mathcal{T}}^{C_i}(t) = c_{1,i} + c_{2,i}(t - t_i) + c_{3,i}(t - t_i)^2 + c_{4,i}(t - t_i)^3$, (for $t \in [t_i, t_{i+2}]$) satisfies (for $i = 0, 1, 2, \ldots, n-1$; $c_{j,i} \in \mathbb{R}^m$, where $j = 1, 2, 3, 4$) $\gamma_{\mathcal{T}}^{C_i}(t_{i+k}) = x_{i+k}$ and $\dot{\gamma}_{\mathcal{T}}^{C_i}(t_{i+k}) = v_{i+k}$, for $k = 0, 1$ with the velocities $v_0, v_1, \ldots, v_{n-1}, v_n \in \mathbb{R}^m$ assumed to be temporarily free parameters (*if unknown*). The coefficients $c_{j,i}$ read (with $\Delta t_i = t_{i+1} - t_i$):

$$c_{1,i} = x_i, \qquad\qquad\qquad c_{2,i} = v_i ,$$
$$c_{4,i} = \frac{v_i + v_{i+1} - 2\frac{x_{i+1}-x_i}{\Delta t_i}}{(\Delta t_i)^2} , \qquad c_{3,i} = \frac{\frac{(x_{i+1}-x_i)}{\Delta t_i} - v_i}{\Delta t_i} - c_{4,i}\Delta t_i . \quad (2)$$

The latter follows from Newton's divided differences formula (see e.g. [1, Chap. 1]). Adding $n-1$ constraints $\ddot{\gamma}_{\mathcal{T}}^{C_{i-1}}(t_i) = \ddot{\gamma}_{\mathcal{T}}^{C_i}(t_i)$ for continuity of $\ddot{\gamma}_{\mathcal{T}}^C$ at $x_1, \ldots, x_{n-1}$ (with $i = 1, 2, \ldots, n-1$) leads by (2) (for $\gamma_{\mathcal{T}}^{C_i}$) to the m tridiagonal linear systems (strictly diagonally dominant) of $n-1$ equations in $n+1$ vector unknowns representing velocities at $\mathcal{M}$ i.e. $v_0, v_1, v_2, \ldots, v_{n-1}, v_n \in \mathbb{R}^m$:

$$v_{i-1}\Delta t_i + 2v_i(\Delta t_{i-1} + \Delta t_i) + v_{i+1}\Delta t_{i-1} = b_i ,$$
$$b_i = 3(\Delta t_i \frac{x_i - x_{i-1}}{\Delta t_{i-1}} + \Delta t_{i-1}\frac{x_{i+1} - x_i}{\Delta t_i}) . \quad (3)$$

(i) Both v_0 and v_n (*if unknown*) can be e.g. calculated from $a_0 = \ddot{\gamma}_{\mathcal{T}}^C(0) = a_n = \ddot{\gamma}_{\mathcal{T}}^C(T_c) = \mathbf{0}$ combined with (2) (this yields *a natural cubic spline interpolant* $\gamma_{\mathcal{T}}^{NS}$ - a special $\gamma_{\mathcal{T}}^C$) which supplements (3) with two missing vector linear equations:

$$2v_0 + v_1 = 3\frac{x_1 - x_0}{\Delta t_0} \ , \quad v_{n-1} + 2v_n = 3\frac{x_n - x_{n-1}}{\Delta t_{n-1}} \ . \tag{4}$$

The resulting m linear systems, each of size $(n+1) \times (n+1)$, (based on (3) and (4)) as strictly row diagonally dominant result in one solution $v_0, v_1, \ldots, v_{n-1}, v_n$ (solved e.g. by Gauss elimination without pivoting - see [1, Chap. 4]), which when fed into (2) determines explicitly *a natural cubic spline* $\gamma_{\mathcal{T}}^{NS}$ (with fixed $\mathcal{T}$). A similar approach follows for arbitrary a_0 and a_n.

(ii) If both v_0 and v_n are given then the so-called *complete spline* $\gamma_{\mathcal{T}}^{CS}$ can be found with $v_1, \ldots v_{n-1}$ determined solely by (3).

(iii) If one of v_0 or v_n is unknown, this can be compensated by setting the respective terminal acceleration e.g. to $\mathbf{0}$. The above scheme relies on solving (3) with one equation from (4). Such splines are denoted here by $\gamma_{\mathcal{T}}^{v_n}$ or $\gamma_{\mathcal{T}}^{v_0}$. Two *non-generic* cases of *Leap-Frog* optimizations deal with the latter.

By (1) $\mathcal{J}_{\mathcal{T}}(\gamma_{\mathcal{T}}^{NS}) = 4\sum_{i=0}^{n-1}(\|c_{3,i}\|^2 \Delta t_i + 3\|c_{4,i}\|^2(\Delta t_i)^3 + 3\langle c_{3,i}|c_{4,i}\rangle(\Delta t_i)^2)$, which ultimately reformulates into (see [2]):

$$\mathcal{J}_T(\gamma_{\mathcal{T}}^{NS}) = 4\sum_{i=0}^{n-1}\Big(\frac{-1}{(\Delta t_i)^3}(-3\|x_{i+1} - x_i\|^2 + 3\langle v_i + v_{i+1}|x_{i+1} - x_i\rangle\Delta t_i$$
$$-(\|v_i\|^2 + \|v_{i+1}\|^2 + \langle v_i|v_{i+1}\rangle)(\Delta t_i)^2\Big) . \tag{5}$$

As mentioned before for fixed knots $\mathcal{T}$, the natural spline $\gamma_{\mathcal{T}}^{NS}$ minimizes (1) (see [1]). Thus upon relaxing the internal knots $\mathcal{T}_{int}$ the original infinite dimensional optimization (1) reduces into finding the corresponding *optimal knots* $(t_1^{opt}, t_2^{opt}, \ldots, t_{n-1}^{opt})$ for (5) (viewed from now on as a multivariate function $J_0(t_1, t_2, \ldots, t_{n-1})$) subject to $t_0 = 0 < t_1^{opt} < t_2^{opt} < \cdots < t_{n-1}^{opt} < t_n = T$. Such reformulated non-linear optimization task (5) transformed into minimizing $J_0(\mathcal{T}_{int})$ (here $t_0 = 0$ and $t_n = T$) forms a difficult task for critical points examination as well as for the numerical computations (see e.g. [2,3,7]). One of the computationally feasible schemes handling (5) is *a Leap-Frog Algorithm*. For optimizing J_0 this scheme is based on the sequence of single variable iterative optimization which in k-th iteration minimizes $J_0^{(k,i)}(s) = \int_{t_{i-1}^k}^{t_{i+1}^{k-1}}\|\ddot{\gamma}_{k,i}^{CS}(s)\|^2 ds$, over $I_i^{k-1} = [t_{i-1}^k, t_{i+1}^{k-1}]$. Here t_i^k is set to be a free variable denoted as s_i. The complete spline $\gamma_{k,i}^{CS} : I_i^{k-1} \to \mathbb{E}^m$ is determined by $\{t_{i-1}^k, s_i, t_{i+1}^{k-1}\}$, both velocities $\{v_{i-1}^k, v_{i+1}^{k-1}\}$ and the interpolation points $\{x_{i-1}, x_i, x_{i+1}\}$. Once s_i^{opt} is found one updates t_i^{k-1} with $t_i^k = s_i^{opt}$ and v_i^{k-1} with the $v_i^k = \dot{\gamma}_{k,i}^{CS}(s_i^{opt})$. Next we pass to the shifted overlapped sub-interval $I_{i+1}^k = [t_i^k, t_{i+2}^{k-1}]$ and repeat the previous step of updating t_{i+1}^{k-1}. Note that both cases $[0, t_2^{k-1}]$ and $[t_{n-2}^{k-1}, T]$ rely on splines discussed in *(iii)*, where the vanishing acceleration replaces one of the velocities v_0^{k-1} or v_n^{k-1}. Once t_{n-1}^{k-1} is changed over the last sub-interval $I_{n-1}^{k-1} = [t_{n-2}^k, T]$

the k-th iteration is terminated and the next local optimization over $I_1^k = [0, t_2^k]$ represents the beginning of the $(k+1)$-st iteration of *Leap-Frog*. The initialization of $\mathcal{T}_{int}$ for *Leap-Frog* can follow normalized *cumulative chord parameterization* (see e.g. [9]) which sets $t_0^0 = 0, t_1^0, \ldots, t_{n-1}^k, t_n^0 = T$ according to $t_0^0 = 0$ and $t_{i+1}^0 = \|x_{i+1} - x_i\| \frac{T}{\hat{T}} + t_i^0$, for $i = 0, 1, \ldots, n - 1$ and $\hat{T} = \sum_{i=0}^{n-1} \|x_{i+1} - x_i\|$.

3   Non-generic Case: First Acceleration and Last Velocity

Let for $x_0, x_1, x_2 \in \mathcal{M}$ (for $n \geq 3$) the corresponding knots (see [1]) t_0 and t_2 be somehow given together with the respective first acceleration and the last velocity $a_0, v_2 \in \mathbb{R}^m$ (without loss $t_0 = 0$). We construct now a C^2 piecewise cubic $\gamma_0^c : [t_0, t_2] \to \mathbb{E}^m$ depending on varying $t_1 \in (t_0, t_2)$ (i.e. a cubic on each $[t_0, t_1]$ and $[t_1, t_2]$) satisfying $\gamma_0^c(t_j) = x_j$ (for $j = 0, 1, 2$), $\ddot{\gamma}_0^c(t_0) = a_0$ and $\dot{\gamma}_0^c(t_2) = v_2$. With $\phi_0 : [t_0, t_2] \to [0, 1]$ (with $\phi_0(t) = (t - t_0)(t_2 - t_0)^{-1}$) the re-parameterized curve $\tilde{\gamma}_0^c = \gamma_0^c \circ \phi_0^{-1} : [0, 1] \to \mathbb{E}^m$ satisfies, for $0 < s_1 < 1$ (where $s_1 = \phi_0(t_1)$): $\tilde{\gamma}_0^c(0) = x_0$, $\tilde{\gamma}_0^c(s_1) = x_1$ and $\tilde{\gamma}_0^c(1) = x_2$, with the adjusted $\tilde{a}_0, \tilde{v}_2 \in \mathbb{R}^m$ equal to:

$$\tilde{a}_0 = \tilde{\gamma}_0^{c''}(0) = (t_2 - t_0)^2 a_0 \,, \quad \tilde{v}_2 = \tilde{\gamma}_0^{c'}(1) = (t_2 - t_0) v_2 \,. \tag{6}$$

An easy inspection shows (for each $s_1 = \phi_0(t_1)$):

$$\tilde{\mathcal{E}}_0(s_1) = \int_0^1 \|\tilde{\gamma}_0^{c''}(s)\|^2 ds = (t_2 - t_0)^3 \int_{t_0}^{t_2} \|\ddot{\gamma}_0^c(t)\|^2 dt = (t_2 - t_0)^3 \mathcal{E}_0(t_1) \,. \tag{7}$$

Thus critical points s_1^{crit} of $\tilde{\mathcal{E}}_0$ are mapped (and vice versa) onto the corresponding critical points $t_1^{crit} = \phi_0^{-1}(s_1^{crit}) = s_1^{crit}(t_2 - t_0) + t_0$ of $\mathcal{E}_0$. Hence optimal points of $\tilde{\mathcal{E}}_0$ and $\mathcal{E}_0$ satisfy $t_1^{opt} = \phi_0^{-1}(s_1^{opt})$. Thus by (7) to decrease $\mathcal{E}_0$ it suffices to decrease $\tilde{\mathcal{E}}_0$. To find the expression for $\tilde{\mathcal{E}}_0$ we determine $\tilde{\gamma}_0^c$ (depending on s_1)

$$\tilde{\gamma}_0^c(s) = \begin{cases} \tilde{\gamma}_0^{lc}(s) \,, & \text{for } s \in [0, s_1] \\ \tilde{\gamma}_0^{rc}(s) \,, & \text{for } s \in [s_1, 1] \end{cases} \tag{8}$$

with $c_{0j}, d_{0j} \in \mathbb{R}^m$ and $\tilde{\gamma}_0^{lc}(s) = c_{00} + c_{01}(s - s_1) + c_{02}(s - s_1)^2 + c_{03}(s - s_1)^3$ and $\tilde{\gamma}_0^{rc}(s) = d_{00} + d_{01}(s - s_1) + d_{02}(s - s_1)^2 + d_{03}(s - s_1)^3$, the following holds:

$$\tilde{\gamma}_0^{lc}(0) = x_0 \,, \quad \tilde{\gamma}_0^{lc}(s_1) = \tilde{\gamma}_0^{rc}(s_1) = x_1 \,, \quad \tilde{\gamma}_0^{rc}(1) = x_2 \,, \tag{9}$$

$$\tilde{\gamma}_0^{lc''}(0) = \tilde{a}_0 \,, \quad \tilde{\gamma}_0^{rc'}(1) = \tilde{v}_2 \,, \tag{10}$$

together with the smoothness (C^1 and C^2) constraints at $s = s_1$ i.e.:

$$\tilde{\gamma}_0^{lc'}(s_1) = \tilde{\gamma}_0^{rc'}(s_1) \,, \quad \tilde{\gamma}_0^{lc''}(s_1) = \tilde{\gamma}_0^{rc''}(s_1) \,. \tag{11}$$

We may assume that (upon shifting the origin of coordinate system) $\tilde{x}_0 = x_0 - x_1$, $\tilde{x}_1 = \mathbf{0}$, $\tilde{x}_2 = x_2 - x_1$ and therefore by (9) we have

$$\tilde{\gamma}_0^c(0) = \tilde{x}_0 \,, \quad \tilde{\gamma}_0^c(s_1) = \mathbf{0} \,, \quad \tilde{\gamma}_0^c(1) = \tilde{x}_2 \,. \tag{12}$$

In sequel, combining (11) with $\tilde{x}_1$ vanishing gives

$$\tilde{\gamma}_0^{lc}(s) = c_{01}(s - s_1) + c_{02}(s - s_1)^2 + c_{03}(s - s_1)^3 \ ,$$
$$\tilde{\gamma}_0^{rc}(s) = c_{01}(s - s_1) + c_{02}(s - s_1)^2 + d_{03}(s - s_1)^3 \ , \tag{13}$$

with $c_{00} = d_{00} = \mathbf{0}$. The unknown vectors $c_{01}, c_{02}, c_{03}, d_{03}$ are determined by solving the system of four linear vector equations obtained from (10) and (12):

$$\tilde{x}_0 = -c_{01}s_1 + c_{02}s_1^2 - c_{03}s_1^3 \ ,$$
$$\tilde{x}_2 = c_{01}(1 - s_1) + c_{02}(1 - s_1)^2 + d_{03}(1 - s_1)^3 \ ,$$
$$\tilde{a}_0 = 2c_{02} - 6c_{03}s_1 \ ,$$
$$\tilde{v}_2 = c_{01} + 2c_{02}(1 - s_1) + 3d_{03}(1 - s_1)^2 \ . \tag{14}$$

An inspection reveals that:

$$c_{01} = \frac{s_1^2\tilde{a}_0 + 2s_1^3\tilde{a}_0 - s_1^4\tilde{a}_0 + 4s_1^2\tilde{v}_2 - 4s_1^3\tilde{v}_2 + 6\tilde{x}_0 - 12s_1\tilde{x}_0 + 6s_1^2\tilde{x}_0 - 12s_1^2\tilde{x}_2}{2s_1(s_1^2 + 2s_1 - 3)} \ ,$$

$$c_{02} = -\frac{-s_1^2\tilde{a}_0 + s_1^3\tilde{a}_0 - 3s_1\tilde{v}_2 + 3s_1^2\tilde{v}_2 + 6\tilde{x}_0 - 6s_1\tilde{x}_0 + 9s_1\tilde{x}_2}{s_1(s_1 - 1)(s_1 + 3)} \ ,$$

$$c_{03} = -\frac{-s_1\tilde{a}_0 + s_1^3\tilde{a}_0 - 2s_1\tilde{v}_2 + 2s_1^2\tilde{v}_2 + 4\tilde{x}_0 - 4s_1\tilde{x}_0 + 6s_1\tilde{x}_2}{2s_1^2(s_1^2 + 2s_1 - 3)} \ ,$$

$$d_{03} = -\frac{s_1^2\tilde{a}_0 - 2s_1^3\tilde{a}_0 + s_1^4\tilde{a}_0 + 6s_1\tilde{v}_2 - 8s_1^2\tilde{v}_2 + 2s_1^3\tilde{v}_2 - 6\tilde{x}_0 + 12s_1\tilde{x}_0 - 6s_1^2\tilde{x}_0}{2s_1(s_1 + 3)(s_1 - 1)^3}$$
$$- \frac{-12s_1\tilde{x}_2 + 8s_1^2\tilde{x}_2}{2s_1(s_1 + 3)(s_1 - 1)^3} \tag{15}$$

satisfy (14) (as functions in s_1). As $\|\tilde{\gamma}_0^{lc''}(s)\|^2 = 4\|c_{02}\|^2 + 24\langle c_{02}|c_{03}\rangle(s - s_1) + 36\|c_{03}\|^2(s - s_1)^2$, $\|\tilde{\gamma}_0^{rc''}(s)\|^2 = 4\|c_{02}\|^2 + 24\langle c_{02}|d_{03}\rangle(s - s_1) + 36\|d_{03}\|^2(s - s_1)^2$:

$$\tilde{\mathcal{E}}_0(s_1) = \int_0^{s_1} \|\tilde{\gamma}_0^{lc''}(s)\|^2 ds + \int_{s_1}^1 \|\tilde{\gamma}_0^{rc''}(s)\|^2 ds = I_1 + I_2,$$

where $I_1 = 4(\|c_{02}\|^2 s_1 - 3\langle c_{02}|c_{03}\rangle s_1^2 + 3\|c_{03}\|^2 s_1^3)$ and $I_2 = 4(\|c_{02}\|^2(1 - s_1) + 3\langle c_{02}|d_{i3}\rangle(1 - s_1)^2 + 3\|d_{03}\|^2(1 - s_1)^3)$. The latter combined with $a_0 = \mathbf{0}$ (and $\tilde{a}_0 = \mathbf{0}$ - see (6)), (13) and (15) yields (with *Mathematica Integrate* and *FullSimplify*):

$$\tilde{\mathcal{E}}_0(s_1) = \frac{-1}{(s_1 + 3)s_1^2(s_1 - 1)^3}(12(-\|\tilde{x}_0\|^2(s_1 - 1)^3 + s_1(\|\tilde{x}_2\|^2(3 - 2s_1)s_1$$
$$+ \|\tilde{v}_2\|^2(s_1 - 1)^2 s_1 + (s_1 - 1)^3\langle\tilde{v}_2|\tilde{x}_0\rangle - (s_1 - 3)(s_1 - 1)s_1\langle\tilde{v}_2|\tilde{x}_2\rangle$$
$$+ 3(s_1 - 1)^2\langle\tilde{x}_0|\tilde{x}_2\rangle))) \ . \tag{16}$$

Note also that $\lim_{s_1 \to 0^+} \tilde{\mathcal{E}}_0(s_1) = (12\|\tilde{x}_0\|^2/0^+) = +\infty$, and $\lim_{s_1 \to 1^-} \tilde{\mathcal{E}}_0(s_1) = (12\|\tilde{x}_2\|^2/0^+) = +\infty$. Hence as $\tilde{\mathcal{E}}_0 \geq 0$ and $\tilde{\mathcal{E}}_0 \in C^1$ the global minimum $s_1^{opt} \in$

$(0, 1)$ exists (one of critical points of $\tilde{\mathcal{E}}_0$). Note that $x_i \neq x_{i+1}$ yields $\|\tilde{x}_0\| \neq 0$ and $\|\tilde{x}_2\| \neq 0$. An inspection shows that (or differentiate symbolically in *Mathematica* $\tilde{\mathcal{E}}_0$ and use *FullSimplify*):

$$\tilde{\mathcal{E}}'_0(s_1) = \frac{1}{(s_1 - 1)^4 s_1^3 (s_1 + 3)^2} (12(2\|\tilde{v}_2\|^2 (s_1 - 1)^2 s_1^3 (s_1 + 1) - 6\|\tilde{x}_2\|^2 s_1^3 (s_1^2 - 3)$$
$$- 3\|\tilde{x}_0\|^2 (s_1 - 1)^4 (s_1 + 2) + (s_1 - 1)^4 s_1 (2s_1 + 3) \langle \tilde{v}_2 | \tilde{x}_0 \rangle$$
$$- 2(s_1 - 1) s_1^3 (-6 + (-3 + s_1) s_1) \langle \tilde{v}_2 | \tilde{x}_2 \rangle$$
$$+ 3(s_1 - 1)^2 s_1 (-3 + s_1 (4 + 3s_1)) \langle \tilde{x}_0 | \tilde{x}_2 \rangle)) . \tag{17}$$

The numerator of (17) is the polynomial of degree 6 i.e. $N_0(s_1) = b_0^0 + b_1^0 s_1 + b_2^0 s_1^2 + b_3^0 s_1^3 + b_4^0 s_1^4 + b_5^0 s_1^5 + b_6^0 s_1^6$, with the coefficients $b_j^0 \in \mathbb{R}$ (for $j = 0, 1, \ldots, 6$) equal to (use e.g. *Mathematica* functions *Factor* and *CoefficientList*): $\frac{b_0^0}{12} = -6\|\tilde{x}_0\|^2$, $\frac{b_1^0}{12} = 21\|\tilde{x}_0\|^2 + 3\langle \tilde{v}_2 | \tilde{x}_0 \rangle - 9\langle \tilde{x}_0 | \tilde{x}_2 \rangle$, $\frac{b_2^0}{12} = -24\|\tilde{x}_0\|^2 - 10\langle \tilde{v}_2 | \tilde{x}_0 \rangle + 30\langle \tilde{x}_0 | \tilde{x}_2 \rangle$, $\frac{b_3^0}{12} = 2\|\tilde{v}_2\|^2 + 6\|\tilde{x}_0\|^2 + 18\|\tilde{x}_2\|^2 + 10\langle \tilde{v}_2 | \tilde{x}_0 \rangle - 12\langle \tilde{v}_2 | \tilde{x}_2 \rangle - 24\langle \tilde{x}_0 | \tilde{x}_2 \rangle$, $\frac{b_4^0}{12} = -2\|\tilde{v}_2\|^2 + 6\|\tilde{x}_0\|^2 + 6\langle \tilde{v}_2 | \tilde{x}_2 \rangle - 6\langle \tilde{x}_0 | \tilde{x}_2 \rangle$, $\frac{b_5^0}{12} = -2\|\tilde{v}_2\|^2 - 3\|\tilde{x}_0\|^2 - 6\|\tilde{x}_2\|^2 - 5\langle \tilde{v}_2 | \tilde{x}_0 \rangle + 8\langle \tilde{v}_2 | \tilde{x}_2 \rangle + 9\langle \tilde{x}_0 | \tilde{x}_2 \rangle$ and $\frac{b_6^0}{12} = 2\|\tilde{v}_2\|^2 + 2\langle \tilde{v}_2 | \tilde{x}_0 \rangle - 2\langle \tilde{v}_2 | \tilde{x}_2 \rangle$.

In a search for a global optimum of $\tilde{\mathcal{E}}_0$, instead of performing any iterative optimization scheme (relying on initial guess), one can invoke *Mathematica Package Solve* which easily finds all roots (real and complex) for a given low order polynomial in one variable. Upon computing the roots of $N_0(s_1)$ we select only these which are real and belong to $(0, 1)$. Next we evaluate $\tilde{\mathcal{E}}_0$ on each critical point $s_1^{crit} \in (0, 1)$ and choose s_1^{crit} with minimal energy $\tilde{\mathcal{E}}_0$ as optimal. Again this particular property of optimizing $\tilde{\mathcal{E}}_0$ is very useful for future Leap-Frog Algorithm as compared with optimizing multiple variable function (5). We analyze in the next section the character of the energy $\tilde{\mathcal{E}}_0$ for the special case (18).

The case of *first velocity and last acceleration given* (covering the last three interpolation points $x_{n-2}, x_{n-1}, x_n \in \mathcal{M}$) is symmetric and as such is omitted.

4   Special Conditions for Non-generic Case of Leap-Frog

For a global minimum of $\tilde{\mathcal{E}}_0$ the analysis of $\tilde{\mathcal{E}}'_0(s_1) = 0$ reduces into finding all real roots of the sixth order polynomial $N_0(s_1)$. Consider a special case of $\tilde{x}_0, \tilde{x}_1, \tilde{x}_2 \in \mathbb{E}^m$ and $\tilde{v}_2 \in \mathbb{R}^m$ which satisfy (for some $k \neq 0$ as $\tilde{x}_0 \neq \mathbf{0}$):

$$\tilde{x}_2 - \tilde{x}_0 = \tilde{v}_2 \qquad \tilde{x}_0 = k\tilde{x}_2 . \tag{18}$$

Remark 1. The case of $k < 0$ yields the so-called *co-linearly ordered data* $\tilde{x}_0, \tilde{x}_1, \tilde{x}_2$. Here the function $x(s) = s\tilde{x}_2 + (1 - s)\tilde{x}_0$ (with $s \in (0, 1)$) satisfies required constraints (18), namely: $x(0) = \tilde{x}_0$, $x(1) = \tilde{x}_2$, $x'(1) = \tilde{x}_2 - \tilde{x}_0 = \tilde{v}_2$, and $x''(0) = \mathbf{0}$. For $k \neq 0$ the normalized cumulative chord reads

$$\hat{s}_1^{cc} = \hat{s}_1^{cc}(k) = \frac{\|\tilde{x}_0\|}{\|\tilde{x}_2\| + \|\tilde{x}_0\|} = \frac{|k|}{1 + |k|}. \tag{19}$$

Noticeably, $\|\tilde{x}_2\| \neq 0$ and $\|\tilde{x}_0\| \neq 0$ as $x_0 \neq x_1$ and $x_1 \neq x_2$. Thus since $|k| = -k$ (for $k < 0$) by (18) we have $x\left(\frac{|k|}{1+|k|}\right) = \tilde{x}_2 \frac{|k|}{1+|k|} + \tilde{x}_0 \frac{1}{1+|k|} = \tilde{x}_2\left(\frac{|k|}{1+|k|} + \frac{k}{1+|k|}\right) = \mathbf{0} = \tilde{x}_1$. Hence the interpolation condition $x(s_1) = \mathbf{0}$ is satisfied with $s_1 = \hat{s}_1^{cc}$. In sequel since $\|x''(s)\| = 0$ over $(0, 1)$, the integral (7) vanishes with $s = \hat{s}_1^{cc}$. Thus $\hat{s}_1^{cc}$ is a global minimizer of $\tilde{\mathcal{E}}_0$ for any $k < 0$. This does not hold for $k > 0$. Note that for n big the case $k > 0$ prevails. $\qquad\square$

By (18) we have $\|\tilde{x}_0\|^2 = k^2\|\tilde{x}_2\|^2$, $\|\tilde{v}_2\|^2 = (1-k)^2\|\tilde{x}_2\|^2$, $\langle\tilde{v}_2|\tilde{x}_2\rangle = (1-k)\|\tilde{x}_2\|^2$, $\langle\tilde{v}_2|\tilde{x}_0\rangle = (k-k^2)\|\tilde{x}_2\|^2$, $\langle\tilde{x}_0|\tilde{x}_2\rangle = k\|\tilde{x}_2\|^2$. Substituting the latter into (16) yields (upon using e.g. *FullSimplify* in *Mathematica*) $\tilde{\mathcal{E}}_0(s) = \tilde{\mathcal{E}}_0^d(s) = (-12(\|\tilde{x}_2\|(k+s(1-k)))^2)/((s-1)^3 s^2(3+s))$. The latter vanishes iff $s = -k/(1-k)$ which for $k < 0$ reads as $s = |k|/(1+|k|) = \hat{s}_1^{cc}(k)$ (as previously $\hat{s}_1^{cc}$ can be treated as a function in k). In a search for other critical points of $\tilde{\mathcal{E}}_0^d$, the respective derivative $\tilde{\mathcal{E}}_0^{d'}$ (e.g. use symbolic differentiation in *Mathematica* and *FullSimplify*) reads:

$$\tilde{\mathcal{E}}_0^{d'}(s) = \frac{24\|\tilde{x}_2\|^2(k+s(1-k))(-3k+6ks+s^2(4-k)+s^3(2-2k))}{(s-1)^4 s^3(3+s)^2} \ . \quad (20)$$

If $k \neq 1$ (i.e. $\tilde{x}_2 \neq \tilde{x}_0$) the first numerator's factor of (20) yields exactly one root $\hat{s}_1^L = -k/(1-k)$. Only for $k < 0$ we have $\hat{s}_1^L \in (0, 1)$. Otherwise for $k > 1$ we have $\hat{s}_1^L > 1$ and for $0 < k < 1$ we have $\hat{s}_1^L < 0$. The analysis of $k < 0$ and $k > 0$ (with $k \neq 1$) for the second cubic factor in (20) is performed below. Note that with $k = 1$ the first linear factor in (20) has no roots and the second cubic factor reduces in quadratic with the roots $\hat{s}_1^{\pm} = -1 \pm \sqrt{2}$. Only $\hat{s}_1 = \hat{s}_1^+ \in (0, 1)$.

(i) Assume that $k < 0$ (the data are co-linearly ordered). The latter shows that cumulative chord $\hat{s}_1^{cc}$ (see the linear factor in (20)) is a critical point of $\tilde{\mathcal{E}}_0^d$.

To find the remaining critical points of $\tilde{\mathcal{E}}_0^d$ the real roots of $M_0(s) = -3k + 6ks + s^2(4-k) + s^3(2-2k)$ over $(0, 1)$ are to be examined. Note that as $M_0(0) = -3k > 0$ (as $k < 0$) and $M_0(1) = 6 > 0$ for the existence of one critical point $\hat{s}_1$ of $\tilde{\mathcal{E}}_0'$ (i.e. here with $\hat{s}_1 = \hat{s}_1^{cc}$) it suffices to show that M_0 is positive at any of its critical points $\hat{u}_0 \in (0, 1)$ (i.e. at points where $M_0'(\hat{u}_0) = 0$ with $M_0(\hat{u}_0) > 0$). Indeed $M_0'(u) = 0$ iff $3k + u(4-k) + u^2(3-3k) = 0$. The discriminant (as $k < 0$) $\bar{\Delta}(k) = 16 - 44k + 37k^2 > 0$ and thus there are two different real roots $\hat{u}_0^-$ and $\hat{u}_0^+$ (both depending on parameter $k < 0$). Since $(-k)/(k-1) < 0$ (again as $k < 0$) by Vieta's formula both roots are of opposite signs. Thus as

$$\hat{u}_0^{\pm} = \hat{u}_0^{\pm}(k) = \frac{k - 4 \pm \sqrt{\Delta}}{6(1-k)} \quad (21)$$

we have $\hat{u}_0^- < 0$ (since for $k < 0$ we have $k - 4 - \sqrt{\Delta} < 0$ and $6(1-k) > 0$). Hence $\hat{u}_0^+ > 0$ - this can be independently shown as being equivalent to true inequality $36k(k-1) > 0$. But as $M_0'(0) = 6k < 0$ and $M_0'(1) = 14 - 2k > 0$ by Intermediate Value Theorem we have that $\hat{u}_0^+ \in (0, 1)$ (and it is a unique root of $M_0'(u) = 0$ over $(0, 1)$). As also $M_0'(0) < 0$ for $u \in (0, \hat{u}_0^+)$ and $M_0'(0) > 0$ for $\hat{u} \in (u_0^+, 1)$ we have minimum of M_0 at $\hat{u}_0^+$ over interval

$(0, 1)$. Evaluating $M_0(\hat{u}_0^+(k))$ (see (21)) yields a function $\bar{M}_0(k) = M_0(\hat{u}_0^+(k))$ in k (again use. e.g. *Mathematica FullSimplify* and *Factor*) which reads: $\bar{M}_0(k) = \frac{-1}{54(k-1)^2}(-64 + 426k - 606k^2 + 217k^3 + 16\sqrt{\bar{\Delta}(k)} - 44k\sqrt{\bar{\Delta}(k)} + 37k^2\sqrt{\bar{\Delta}(k)})$. By Taylor expansion we have $f(x) = \sqrt{1+x} = 1 + (1/2)x + (-1/(2(1+\xi)^{3/2}))x^2$ (with $0 < \xi < x$ if $x > 0$ and $x < \xi < 0$ if $x < 0$). Upon applying the latter to $\sqrt{\bar{\Delta}(k)} = 4\sqrt{1 + (37/16)k^2 - (11/4)k}$ with $x = (37/16)k^2 - (11/4)k$ we arrive at $\lim_{k\to 0^-} \bar{M}_0(k) = 0$. Again by Taylor expansion, the domineering factor (recall for $k \approx O^-$ we have $|k| \geq |k|^\alpha$ with $\alpha \geq 1$) in the expression for $M_0(k)$ (inside the brackets) is a linear component $426k - 88k - 176k = 162k < 0$, as $k < 0$ - (here the constant 64 is canceled). Thus $\bar{M}_0(k) > 0$, for sufficiently small $k < 0$. To show that $\lim_{k\to-\infty} \bar{M}_0(k) = -\infty$, it suffices to show $\lim_{k\to-\infty}((217k^3 + 37k^2\sqrt{\bar{\Delta}(k)})/(k-1)^2) = +\infty$. The latter follows upon observation that (for $k < 0$) $217k^3 + 37k^2\sqrt{\bar{\Delta}(k)} > 217k^3 + 37k^2\sqrt{36k^2} = 217k^3 + 222k^2|k| = -5k^3$. The *Mathematica* function *NSolve* applied to $\bar{M}_0(k) = 0$ yields two real roots i.e. $k_1 = 0$ (excluded as $\tilde{x}_0 = k\tilde{x}_2$) and $k_2 \approx -26.1326$. Next $\bar{M}_0'(k) = \frac{1}{54(k-1)^3}(-298 + 786k - 651k^2 + 217k^3 + 34\sqrt{\bar{\Delta}(k)} - 89k\sqrt{\bar{\Delta}(k)} + 37k^2\sqrt{\bar{\Delta}(k)})$. Again, *Solve* applied to $\bar{M}_0'(k) = 0$ yields one root -4.61116. Combining the latter with the plotted graph of $\bar{M}_0(k)$ renders for each $k \in (k_2, 0)$ the following: $\bar{M}_0 > 0$ and thus $M_0 > 0$. Hence, for each $k \in (k_2, 0)$ there is only one critical point of $\tilde{\mathcal{E}}_0^d$ over $(0, 1)$ - i.e. cumulative chord $\hat{s}_1^{cc} = |k|/(1 + |k|)$. Hence if any iterative optimization scheme for $\tilde{\mathcal{E}}_0^d$ is invoked a good initial guess can be an arbitrary number from the interval $(0, 1)$ (due to unimodality of $\tilde{\mathcal{E}}_0^d$). In case of small perturbations of (18) one expects that $\tilde{\mathcal{E}}_0^\delta$ preserves a similar pattern as its unperturbed counterpart $\tilde{\mathcal{E}}_0^0 = \tilde{\mathcal{E}}_0^d$ (see Proposition 1). Thus, for arbitrary $k_2 < k < 0$, a good initial guess to optimize $\tilde{\mathcal{E}}_0^\delta$ should be chosen in the proximity of cumulative chord $\hat{s}_1^{cc}(k)$.

Clearly for $k = k_2 \approx -26.1326$ (the second case when $k = 0$ is excluded) $M_0(\hat{u}_0^+(k_2)) = \bar{M}_0(k_2) = 0$ and $M_0'(\hat{u}_0^+(k_2)) = M_0'(k_2) = 0$ (see (21)). Thus we have one additional critical point $\hat{u}_0^+(k_2) \in (0, 1)$ of $\tilde{\mathcal{E}}_0^d$. Hence for k_2 there are exactly two critical points of $\tilde{\mathcal{E}}_0^d$ over $(0, 1)$ - one is a cumulative chord $\hat{s}_1^{cc}(k_2) \in (0, 1)$ (a global minimum) and the second one $\hat{s}_1^0 = u_0^+(k_2) \in (0, 1)$. Substituting $k_2 \approx -26.1326$ into (19) and (21) gives $\hat{u}_0^+(k_2) \approx 0.813606 < \hat{s}_1^{cc}(k_2) = (|k_2|/(1 + |k_2|)) \approx 0.963144$. Of course $u_0^+(k_2)$ must be a a saddle-like point of $\tilde{\mathcal{E}}_0^d$ - recall here that $\tilde{\mathcal{E}}_0^d(\hat{s}_1^{cc}(k_2)) = 0$ (attained global minimum), which is smaller than $\tilde{\mathcal{E}}_0^d(\hat{u}_0^+(k_2)) \approx 12083.9\|\tilde{x}_2\|^2 > 0$ and that $\lim_{s\to 0+} \tilde{\mathcal{E}}_0^d(s) = \lim_{s\to 1+} \tilde{\mathcal{E}}_0^d(s) = +\infty$. This together with non-negativity of $\tilde{\mathcal{E}}_0^d$ and its smoothness over $(0, 1)$ implies that $\hat{u}_0^+(k_2)$ is a saddle-like point of $\tilde{\mathcal{E}}_0^d$. Thus for $k = k_2$ if any iterative optimization scheme for $\tilde{\mathcal{E}}_0^d$ is to be invoked a good initial guess can be an arbitrary number from the interval $(\hat{s}_1^{cc}(k_2), 1)$. As for small perturbations of (18) one expects the energy $\tilde{\mathcal{E}}_0^\delta$ to have as similar pattern as its unperturbed counterpart $\tilde{\mathcal{E}}_0^0 = \tilde{\mathcal{E}}_0^d$. Thus, for $k = k_2$, a good initial guess to optimize $\tilde{\mathcal{E}}_0^\delta$ should also be taken closely to cumulative chord $\hat{s}_1^{cc}(k_2)$ and preferably from $(\hat{s}_1^{cc}(k_2), 1)$.

For $k \in (-\infty, k_2)$ we have $M_0(\hat{u}_0^+(k)) = \bar{M}_0(k) < 0$. Thus for each $k \in (-\infty, k_2)$, as $M_0(0) > 0$, $M_0(1) > 0$, $M_0(\hat{u}_0^+(k)) < 0$ and M_0' vanishes over $(0, 1)$ only at $\hat{u}_0^+(k) \in (0, 1)$, there are exactly two different additional critical points $\hat{s}_0^1(k), s_0^2(k) \in (0, 1)$ (say $\hat{s}_0^1(k) < \hat{s}_0^2(k)$) of $\tilde{\mathcal{E}}_0^d$ (as $M_0(s_0^{1,2}(k)) = 0$). Clearly the inequalities hold $\hat{s}_0^1(k) < \hat{u}_0^+(k) < \hat{s}_0^2(k)$. Recall that the global minimum of $\tilde{\mathcal{E}}_0^d$ is attained at cumulative chord $\hat{s}_1^{cc}$, where $\tilde{\mathcal{E}}_0^d$ vanishes. Note also that here $\hat{s}_1^{cc} \approx 1$ as $\hat{s}_1^{cc}(k) = |k|/(1 + |k|) \in (|k_2|/(1 + |k_2|), 1) = (0.963144, 1)$ for $k \in (-\infty, k_2)$. To show the latter use the facts that $f(x) = (x/(1 + x))$ is increasing and $0 \le f(x) < 1$ for $0 \le x \le 1$ and $\lim_{x \to 1^-} f(x) = 1$. In addition, as $M_0(\hat{s}_1^{cc}(k)) = (3 - 4k)k/(-1 + k)^2 \ne 0$ for $k \in (-\infty, k_2)$, and $M_0(\hat{s}_1^{1,2}(k)) = 0$ we have $\hat{s}_1^{cc}(k) \ne s_0^{1,2}(k)$. In Remark 2 we will show that none of $\hat{s}_0^{1,2}$ can be saddle-like points (for $k \in (-\infty, k_2)$). Thus as $\lim_{s \to 0^+} \tilde{\mathcal{E}}_0^d(s) = \lim_{s \to 1^-} \tilde{\mathcal{E}}_0^d(s) = +\infty$ and $\tilde{\mathcal{E}}_0^d(\hat{s}_1^{cc}(k))$ attains its global minimum both $\hat{s}_0^{1,2}$ must be on one side of $\hat{s}_1^{cc}$ (as otherwise that would imply both $\hat{s}_0^1$ and $\hat{s}_0^2$ to be saddle-like points, since no more than 3 critical points of $\tilde{\mathcal{E}}_0^d$ over $(0, 1)$ exist). Thus to prove that $\hat{u}_0^{1,2}(k) < \hat{s}_1^{cc}(k)$ its suffices to show $\hat{s}_0^1(k) < \hat{s}_1^{cc}(k)$. For the latter (as $\hat{s}_0^1(k) < \hat{u}_0^+(k)$) it is sufficient to prove $\hat{u}_0^+(k) < \hat{s}_1^{cc}(k)$ (where $k \in (-\infty, k_2)$). A simple inspection shows that $\hat{u}_0^+(k) = (4 - k - \sqrt{16 - 44k + 37k^2})/(6(k - 1)) < \hat{s}_1^{cc}(k) = |k|/(1 + |k|)$ holds as this requires $4 - 7k > \sqrt{\Delta}$ which is true since $k(k - 1) > 0$ (with $k < 0$). Thus at $\hat{s}_0^1(k)$ (at $\hat{s}_0^2(k)$) we have a local minimum (maximum) of $\tilde{\mathcal{E}}_0^d$. Again, if any iterative optimization scheme for $\tilde{\mathcal{E}}_0^d$ is invoked a good initial guess can be an arbitrary number from the interval $(\hat{s}_1^{cc}, 1)$. For small perturbations of (18) one expects the energy $\tilde{\mathcal{E}}_0^\delta$ to preserve a pattern of its unperturbed counterpart $\tilde{\mathcal{E}}_0^0 = \tilde{\mathcal{E}}_0^c$ (see Proposition 1). Consequently, for any $k \in (-\infty, -26.1326)$, a good initial guess can be taken as a close to $\hat{s}_1^{cc}(k)$ and from the interval $(\hat{s}_1^{cc}(k), 1)$.

(ii) Assume now that $k > 0$ (the data are *co-linearly unordered*). As here $s_1^L = -k/(1 - k) \notin (0, 1)$ (see (20)) the critical points of $\tilde{\mathcal{E}}_0^d$ coincides with the roots of a cubic $N_c(s) = -3k + 6ks + s^2(4 - k) + s^3(2 - 2k)$.

Evidently for that for $0 < k < 1$ there is only one change of signs of the coefficients (three are positive and one is negative). By Fermat sign principle there exists up to one positive root of $N_c(s)$. The analysis from Sect. 3 assures the existence of at least one critical point of $\tilde{\mathcal{E}}_0$ over $(0, 1)$ ($\tilde{\mathcal{E}}_0^d$ is a special case of $\tilde{\mathcal{E}}_0$). Thus for $0 < k < 1$ there exists exactly one critical point $\hat{s}_1 \in (0, 1)$ (a global minimum) of $\tilde{\mathcal{E}}_0^d$.

The case $k = 1$ (with $\tilde{x}_2 = \tilde{x}_0$) already analyzed yields one critical point $\hat{s}_1 = -1 + \sqrt{2} \in (0, 1)$ of $\tilde{\mathcal{E}}_0^d$.

Finally, for $k > 1$ as $N_c(0) = -3k < 0$, $N_c(1) = 6 > 0$ and $N_c \in C^\infty$, it suffices to show that there is up to one root of $N_c'(u) = 0$, for $u \in (0, 1)$. Of course no roots for $N_c'(u) = 0$ yields strictly increasing $N_c(s)$ over $(0, 1)$ (as $N_c(0) < 0$ and $N_c(1) > 0$) and hence exactly one critical point $\hat{s}_1 \in (0, 1)$ (a global minimum) of $\tilde{\mathcal{E}}_0^d$. The existence of exactly one root $u_1 \in (0, 1)$ for $N_c'(u) = 0$, still yields (since $N_c(0) < 0$ and $N_c(1) > 0$) exactly one root $\hat{s}_1 \in (0, 1)$ of $N_c(s) = 0$ (this time N_c is not monotonic with the exception of the case when $\hat{s}_1 = u_1$, i.e. when u_1 is a saddle-like point of N_c). To show that $N_c'(s) = 6k + 2s(4 - k) + 6s^2(1 - k) = 0$ has up to one root over $(0, 1)$, note

that as now $1 - k < 0$ we have $lim_{s \to \pm\infty} N'_c(s) = -\infty$. The latter combined with $N'_c(0) = 6k > 0$ assures the existence of exactly one negative and one positive root $N'_c(s) = 0$. This completes the proof.

Thus for $k > 0$ the energy $\tilde{\mathcal{E}}_0^d$ *has exactly one critical point* $\hat{s}_1 \in (0, 1)$.

5   Perturbed Special Case

The case when $\{\tilde{x}_0, \tilde{x}_1 = \mathbf{0}, \tilde{x}_2\}$ and $\tilde{v}_2$ do not satisfy (18) is considered now. Upon introducing a perturbation vector $\delta = (\delta_1, \delta_2) \in \mathbb{R}^{2m}$ the question arises whether a unimodality of $\tilde{\mathcal{E}}_0^d = \tilde{\mathcal{E}}_0^{\delta=0}$ (holding for special data (18)) extends to the perturbed case i.e. to $\tilde{\mathcal{E}}_0^\delta$. In doing so, assume the following holds:

$$\tilde{x}_2 - \tilde{x}_0 - \tilde{v}_2 = \delta_1 , \qquad \tilde{x}_0 - k\tilde{x}_2 = \delta_2 , \tag{22}$$

(for some $k \neq 0$) with the corresponding $\tilde{\mathcal{E}}_0^\delta$ derived as in (16) (see also (23)). For $\delta_1 = \delta_2 = \mathbf{0} \in \mathbb{R}^m$ formulas (22) reduce into (18) (i.e. $\tilde{\mathcal{E}}_0^0 = \tilde{\mathcal{E}}_0$ derived for (18)). For an explicit formula of $\tilde{\mathcal{E}}_0^\delta$ and $\tilde{\mathcal{E}}_0^{\delta'}$ we resort to (recalling (22)): $\|\tilde{x}_0\|^2 = k^2\|\tilde{x}_2\|^2 + \|\delta_2\|^2 + 2k\langle\tilde{x}_2|\delta_2\rangle$, $\|\tilde{v}_2\|^2 = (1-k)^2\|\tilde{x}_2\|^2 + \|\delta_1\|^2 + \|\delta_2\|^2 + 2\langle\delta_1|\delta_2\rangle - 2(1-k)\langle\tilde{x}_2|\delta_1\rangle - 2(1-k)\langle\tilde{x}_2|\delta_2\rangle$, $\langle\tilde{v}_2|\tilde{x}_2\rangle = (1-k)\|\tilde{x}_2\|^2 - \langle\tilde{x}_2|\delta_1\rangle - \langle\tilde{x}_2|\delta_2\rangle$, $\langle\tilde{v}_2|\tilde{x}_0\rangle = (k-k^2)\|\tilde{x}_2\|^2 + (1-2k)\langle\tilde{x}_2|\delta_2\rangle - k\langle\tilde{x}_2|\delta_1\rangle - \langle\delta_1|\delta_2\rangle - \|\delta_2\|^2$ and $\langle\tilde{x}_0|\tilde{x}_2\rangle = k\|\tilde{x}_2\|^2 + \langle\tilde{x}_2|\delta_2\rangle$. Substituting the latter into the formula for $\tilde{\mathcal{E}}_0$ (here $s_1 = s$) (see (16)) yields (we use here *Mathematica* function *FullSimplify*)

$$\begin{aligned}\tilde{\mathcal{E}}_0^\delta(s) = {} & \frac{-1}{(s-1)^3 s^2(s+3)}(12(\|\delta_2\|^2(s-1)^2 + k^2\|\tilde{x}_2\|^2(s-1)^2 \\ & + s(\langle\delta_1|\delta_2\rangle(s-1)^2(1+s) + s(\|\tilde{x}_2\|^2 + \|\delta_1\|^2(s-1)^2 + \langle\tilde{x}_2|\delta_1\rangle \\ & - s^2\langle\tilde{x}_2|\delta_1\rangle - 2\langle\tilde{x}_2|\delta_2\rangle) + 2\langle\tilde{x}_2|\delta_2\rangle) + k(s-1)(-2\|\tilde{x}_2\|^2 s \\ & + (s-1)(s(1+s)\langle\tilde{x}_2|\delta_1\rangle + 2\langle\tilde{x}_2|\delta_2\rangle)))))\end{aligned} \tag{23}$$

which upon simplification yields $\tilde{\mathcal{E}}_0^\delta(s) = (-12M_0^\delta(s))/((s-1)^3 s^2(s+3))$, where M_0^δ is the 4-th order polynomial in s with the coefficients (use *Mathematica* functions *Factor* and *CoefficientList*): $a_0^{0,\delta} = \|\delta_2\|^2 + k^2\|\tilde{x}_2\|^2 + 2k\langle\tilde{x}_2|\delta_2\rangle$, $a_1^{0,\delta} = \langle\delta_1|\delta_2\rangle - 2\|\delta_2\|^2 + 2k\|\tilde{x}_2\|^2 - 2k^2\|\tilde{x}_2\|^2 + k\langle\tilde{x}_2|\delta_1\rangle + 2\langle\tilde{x}_2|\delta_2\rangle - 4k\langle\tilde{x}_2|\delta_2\rangle$, $a_2^{0,\delta} = -\langle\delta_1|\delta_2\rangle + \|\delta_1\|^2 + \|\delta_2\|^2 + \|\tilde{x}_2\|^2 - 2k\|\tilde{x}_2\|^2 + k^2\|\tilde{x}_2\|^2 + \langle\tilde{x}_2|\delta_1\rangle - k\langle\tilde{x}_2|\delta_1\rangle - 2\langle\tilde{x}_2|\delta_2\rangle + 2k\langle\tilde{x}_2|\delta_2\rangle$, $a_3^{0,\delta} = -\langle\delta_1|\delta_2\rangle - 2\|\delta_1\|^2 - k\langle\tilde{x}_2|\delta_1\rangle$ and $a_4^{0,\delta} = \langle\delta_1|\delta_2\rangle + \|\delta_1\|^2 - \langle\tilde{x}_2|\delta_1\rangle + k\langle\tilde{x}_2|\delta_1\rangle$ with the corresponding derivative (use symbolic differentiation in *Mathematica* and apply *Factor* and *CoefficientList*) $\tilde{\mathcal{E}}_0^{\delta'}(s) = (12N_0^\delta(s))/((s-1)^4 s^3(s+3)^2)$, where N_0^δ is the 6-th order polynomial in s with the coefficients: $b_0^{0,\delta} = -6\|\delta_2\|^2 - 6k^2\|\tilde{x}_2\|^2 - 12k\langle\tilde{x}_2|\delta_2\rangle$, $b_1^{0,\delta} = -3\langle\delta_1|\delta_2\rangle + 18\|\delta_2\|^2 - 6k\|\tilde{x}_2\|^2 + 18k^2\|\tilde{x}_2\|^2 - 3k\langle\tilde{x}_2|\delta_1\rangle - 6\langle\tilde{x}_2|\delta_2\rangle + 36k\langle\tilde{x}_2|\tilde{\delta}_2\rangle$, $b_2^{0,\delta} = 10\langle\delta_1|\delta_2\rangle - 14\|\delta_2\|^2 + 20k\|\tilde{x}_2\|^2 - 14k^2\|\tilde{x}_2\|^2 + 10k\langle\tilde{x}_2|\delta_1\rangle + 20\langle\tilde{x}_2|\delta_2\rangle - 28k\langle\tilde{x}_2|\delta_2\rangle$, $b_3^{0,\delta} = -6\langle\delta_1|\delta_2\rangle + 2\|\delta_1\|^2 - 2\|\delta_2\|^2 + 8\|\tilde{x}_2\|^2 - 6k\|\tilde{x}_2\|^2 - 2k^2\|x_2\|^2 + 8\langle\tilde{x}_2|\delta_1\rangle - 6k\langle\tilde{x}_2|\delta_1\rangle - 6\langle\tilde{x}_2|\delta_2\rangle - 4k\langle\tilde{x}_2|\delta_2\rangle$, $b_4^{0,\delta} = -4\langle\delta_1|\delta_2\rangle - 2\|\delta_1\|^2 + 4\|\delta_2\|^2 + 4\|\tilde{x}_2\|^2 - 8k\|\tilde{x}_2\|^2 + 4k^2\|\tilde{x}_2\|^2 - 2\langle\tilde{x}_2|\delta_1\rangle - 4k\langle\tilde{x}_2|\delta_1\rangle - 8\langle\tilde{x}_2|\delta_2\rangle + 8k\langle\tilde{x}_2|\delta_2\rangle$,

$b_5^{0,\delta} = \langle\delta_1|\delta_2\rangle - 2\|\delta_1\|^2 - 4\langle\tilde{x}_2|\delta_1\rangle + k\langle\tilde{x}_2|\delta_1\rangle$ and $b_5^{0,\delta} = 2\langle\delta_1|\delta_2\rangle + 2\|\delta_1\|^2 - 2\langle\tilde{x}_2|\delta_1\rangle + 2k\langle\tilde{x}_2|\delta_1\rangle$.

The following result holds (the proof is straightforward):

Proposition 1. *Assume that for unperturbed data* (18) *the corresponding energy* $\tilde{\mathcal{E}}_0^0$ *has exactly one critical point* $\hat{s}_0 \in (0,1)$ *at which* $\tilde{\mathcal{E}}_0^{0''}(\hat{s}_0) > 0$. *Then there exists sufficiently small* $\varepsilon_0 > 0$ *such that for all* $\|\delta\| < \varepsilon_0$ *(where* $\delta = (\delta_1,\delta_2) \in \mathbb{R}^{2m}$) *the perturbed data* (22) *yield the energy* $\tilde{\mathcal{E}}_0^\delta$ *with exactly one critical point* $\hat{s}_0^\delta \in (0,1)$ *(a global minimum* $\hat{s}_0^\delta$ *of* $\tilde{\mathcal{E}}_0^\delta$ *is sufficiently close to* $\hat{s}_0$).

Remark 2. The condition $\tilde{\mathcal{E}}_0^{0'}(s) = \tilde{\mathcal{E}}_0^{0''}(s) = 0$ excludes among all possible saddle-like points of $\tilde{\mathcal{E}}_0^0 = \tilde{\mathcal{E}}_0^d$ (which as shown, e.g. happens for $k = k_2 \approx -26.1326$). In a search for other possible saddle-like points for $k \leq k_2$ varying we eliminate variable s $\tilde{\mathcal{E}}_0^{0'}(s) = 0$ and $\tilde{\mathcal{E}}_0^{0''}(s) = 0$ by resorting to *Mathematica* function *Eliminate*. Indeed upon symbolic differentiation of $\tilde{\mathcal{E}}_0^{\delta'}$ (and then putting $\delta = 0$) with *Mathematica* function *FullSimplify* we obtain $\tilde{\mathcal{E}}_0^{0''}(s) = \frac{-24\|\tilde{x}_2\|^2}{(s-1)^5 s^4 (s+3)^3}(27k^2 + (18k - 102k^2)s + (-72k + 120k^2)s^2 + (96k - 12k^2)s^3 + (46 + 28k - 53k^2)s^4 + (40 - 50k + 10k^2)s^5 + (10 - 20k + 10k^2)s^6$. Using *Eliminate* function in *Mathematica* applied to $\tilde{\mathcal{E}}_0^{0'}(s) = \tilde{\mathcal{E}}_0^{0''}(s) = 0$ (in fact applied to the respective numerators of the first and the second derivatives of $\tilde{\mathcal{E}}_0^0$) leads to $576k^3 - 4209k^4 + 10636k^5 - 11277k^6 + 4152k^7 + 176k^8 = 0$ which when factorized (use e.g. *Mathematica Factor*) equals to $k^3(-3 + 4k)^2(64 - 297k + 276k^2 + 11k^3) = 0$. *Mathematica* function *NSolve* yields four non-negative roots $k = 0$, $k = 3/4$, $k = 0.300288$ and $k = 0.741423$ (excluded as $k \leq k_2$) and one negative $k = -26.1326 = k_2$. The latter is not only consistent with the previous analysis but also implies that the saddle-like point can only occur for $k = k_2$. This fact was used when we analyzed the critical points of $\tilde{\mathcal{E}}_0^0$ for different $k < 0$. $\qquad\square$

Example 1. Let $\tilde{x}_0, \tilde{x}_1 = \mathbf{0}, \tilde{x}_2 \in \mathbb{E}^m$ be *co-linearly ordered* i.e. $\tilde{x}_0 = k\tilde{x}_2$, for some $k < 0$ and $\|\tilde{x}_2\| = 1$. The energy $\tilde{\mathcal{E}}_0^d$ with $\|\tilde{x}_2\| = 1$ reads here as $\tilde{\mathcal{E}}_0^d(s) = (-12((k + s - ks)^2))/((s-1)^3 s^2(3+s))$. The plot of $\tilde{\mathcal{E}}_0^d$ with $k = -4, -15, -25 \in (k_2 \approx -26.1326, 0)$ is shown in Fig. 1. As already proved, in this case there is only *one critical point* of $\tilde{\mathcal{E}}_0^0$ at cumulative chords $\hat{s}_1^{cc}(k) = 4/5 = 0.6$, $\hat{s}_1^{cc}(k) =$
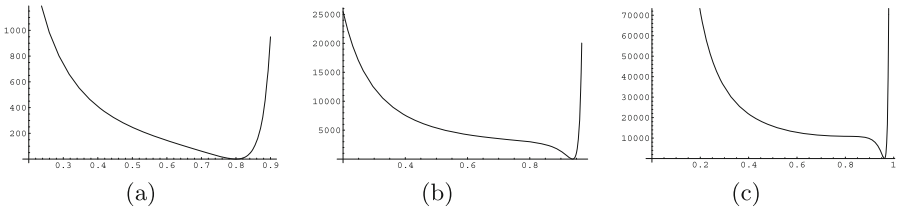

(a)   (b)   (c)

Fig. 1. The graph of $\tilde{\mathcal{E}}_0^d$ for different $\tilde{x}_0, \tilde{x}_1, \tilde{x}_2 \in \mathbb{E}^m$ co-linearly ordered with varying $k \in (k_2, 0)$ and $\|\tilde{x}_2\| = 1$: (a) $k = -4$ and a global minimum at $\hat{s}_1^{cc}(k) = 4/5 = 0.8$, (b) $k = -15$ and a global minimum at $\hat{s}_1^{cc}(k) = 15/16 \approx 0.9375$, (c) $k = -25$ and a global minimum at $\hat{s}_1^{cc}(k) = 25/26 \approx 0.961538$.
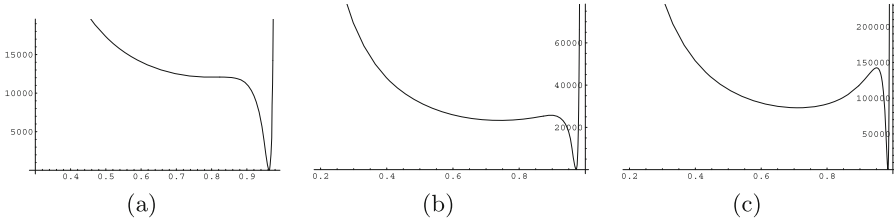
Fig. 2. The graph of $\tilde{\mathcal{E}}_0^d$ for $\tilde{x}_0, \tilde{x}_1, \tilde{x}_2 \in \mathbb{E}^m$ co-linearly ordered with varying $k \in (-\infty, k_2]$ and $\|\tilde{x}_2\| = 1$: (a) $k = k_2$ and a global minimum at $\hat{s}_1^{cc}(k_2) = (|k_2|/(1+|k_2|)) \approx 0.963144$ and saddle-like point at $\hat{s}_1^0(k_2) \approx 0.813607$, (b) $k = -35$ and a global minimum at $\hat{s}_1^{cc}(k) = 35/36 \approx 0.972222$ and two other critical points i.e. with local maximum $\hat{s}_0^2 \approx 0.897748$ and with local minimum $\hat{s}_0^1 \approx 0.743991$, (c) $k = -65$ and global minimum at $\hat{s}_1^{cc}(k) = 65/66 \approx 0.984848$ and two other critical points i.e. with local maximum $\hat{s}_0^2 \approx 0.950547$ and with local minimum $\hat{s}_0^1 \approx 0.711383$.

$15/16 \approx 0.9375$ and $\hat{s}_1^{cc}(k) = 25/26 \approx 0.961538$, respectively (where $\tilde{\mathcal{E}}_0^d(s_1^{cc}(k)) = 0$). Similarly the plot of the corresponding energy $\tilde{\mathcal{E}}_0^d$ with $k = k_2 \approx -26.1326$ is shown in Fig. 2a). Here there are *two critical points* of $\tilde{\mathcal{E}}_0^d$ i.e. a global minimum at cumulative chord $\hat{s}_1^{cc}(k_2) \approx 26.1326/27.1326 \approx 0.963144$ (where $\tilde{\mathcal{E}}_0^d(\hat{s}_1^{cc}(k_2)) = 0$) and a saddle-like point $\hat{s}_1^0(k_2) \approx 0.813607$ (with $\tilde{\mathcal{E}}_0^d(\hat{s}_1^0(k_2)) \approx 12083.9$). Finally, the plot of $\tilde{\mathcal{E}}_0^d$ with $k = -35, -65 \in (-\infty, k_2)$ is shown Fig. 2b)–c). As established above, *a single global minimum* $\tilde{\mathcal{E}}_0^d$ is again taken at cumulative chord $\hat{s}_1^{cc}(k) = 35/36 \approx 0.972222$ (or at $\hat{s}_1^{cc}(k) = 65/66 \approx 0.984848$) with $\tilde{\mathcal{E}}_0^d(\hat{s}_1^{cc}(k)) = 0$. There are *other two critical points*: local maximum at $\hat{s}_0^2(k) \approx 0.897748$ with $\tilde{\mathcal{E}}_0^d(\hat{s}_0^2(k)) \approx 25683.8$ (or at $\hat{s}_0^2(k) \approx 0.950547$ with $\tilde{\mathcal{E}}_0^d(\hat{s}_0^2(k)) \approx 142466$) and local minimum at $\hat{s}_0^1(k) \approx 0.743991$ with $\tilde{\mathcal{E}}_0^d(\hat{s}_0^1(k)) \approx 23297$ (or at $\hat{s}_1^2(k) \approx 0.711383$ with $\tilde{\mathcal{E}}_0^d(\hat{s}_1^2(k)) \approx 86569.7$). Note that for $k = 35, 64$ as already proved the critical points and cumulative chord $\hat{s}_1^{cc}(k)$ satisfy $\hat{s}_0^{1,2}(k) < \hat{s}_1^{cc}(k)$ and $\hat{s}_1^{cc}(k) \approx 1$.

Let now $\tilde{x}_0, \tilde{x}_1 = \mathbf{0}, \tilde{x}_2 \in \mathbb{E}^m$ be *co-linearly unordered* i.e. $\tilde{x}_0 = k\tilde{x}_2$, for some $k > 0$ (here also $\|\tilde{x}_2\| = 1$). The corresponding energy $\tilde{\mathcal{E}}_0^d$ coincides with the one derived for $k < 0$. The plot of $\tilde{\mathcal{E}}_0^d$ with $k = 1/2, 1, 5$ is shown in Fig. 3. As proved for $k > 0$ there is only *one critical point (a global minimum)* of $\tilde{\mathcal{E}}_0^d$ different
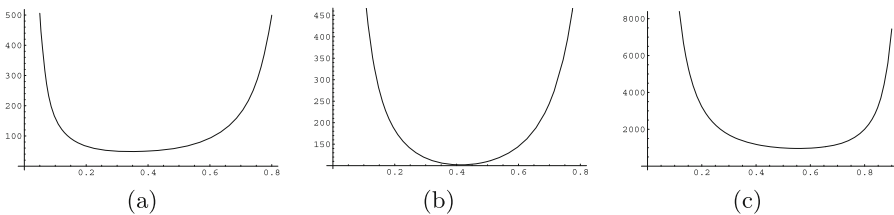

Fig. 3. The graph of $\tilde{\mathcal{E}}_0^d$ for $\tilde{x}_0, \tilde{x}_1, \tilde{x}_2 \in \mathbb{E}^m$ co-linearly unordered with varying $k \in (0, +\infty)$ and $\|\tilde{x}_2\| = 1$: (a) $k = 1/2$ and a global minimum at $\hat{s}_1 \approx 0.346272$ different than $\hat{s}_1^{cc}(k) = (|k|/(1 + |k|)) = 1/3 \approx 0.333333$, (b) $k = 1$ and a global minimum at $\hat{s}_1 = 1 - \sqrt{2} \approx 0.414214$ different than $\hat{s}_1^{cc}(k) = 1/2$, (c) $k = 5$ and global minimum at $\hat{s}_1 \approx 0.556194$ different than $\hat{s}_1^{cc}(k) = 5/6 \approx 0.833333$.

than cumulative chords $\hat{s}_1^{cc}(k) = 1/3 \approx 0.333333$, $\hat{s}_1^{cc}(k) = 1/2$ and $\hat{s}_1^{cc}(k) = 5/6 \approx 0.833333$, respectively. For $k = 0.5$ (see Fig. 3a)) the global minimum $\hat{s}_1 \approx 0.346272$ yields $\tilde{\mathcal{E}}_0^d(\hat{s}_1) \approx 48.5065 < \tilde{\mathcal{E}}_0^d(\hat{s}_1^{cc}) = 48.6$. For $k = 1$ (see Fig. 3b)) the global minimum $\hat{s}_1 \approx 0.414214$ yields $\tilde{\mathcal{E}}_0^d(\hat{s}_1) \approx 101.912 < \tilde{\mathcal{E}}_0^d(\hat{s}_1^{cc}) \approx 109.714$. Note that here as proved $\hat{s}_1 = -1+\sqrt{2}$. Finally, for $k = 5$ (see Fig. 3c)) the global minimum $\hat{s}_1 \approx 0.556194$ yields $\tilde{\mathcal{E}}_0^d(\hat{s}_1) \approx 961.081 < \tilde{\mathcal{E}}_0^d(\hat{s}_1^{cc}) = 2704.7$.

Consider *the unperturbed planar data* $\tilde{x}_2 = (3/5, 4/5)$, $\tilde{x}_0 = (-12/5, -16/5)$, $\tilde{v}_2 = (3, 4)$ clearly satisfying (18) with $k = -4 \in (k_2 \approx -26.1226, 0)$. The graph of $\tilde{\mathcal{E}}_0^0$ is shown in Fig. 1a). We perturb now the co-linearity of $\tilde{x}_0, \tilde{x}_1 = \mathbf{0}, \tilde{x}_2$ by taking $\tilde{x}_0^{\delta_2} = k\tilde{x}_2 + \delta_2 = \tilde{x}_0 + \delta_2$, for some $\delta_2 \in \mathbb{R}^2$ (and any fixed $k < 0$). In this example the second interpolation point $\tilde{x}_2$ remains *fixed* with $\|\tilde{x}_2\| = 1$. Similarly we violate the first condition in (18) by choosing a new velocity $\tilde{v}_2^{\delta_1,\delta_2}$ and perturbation $\delta_1 \in \mathbb{R}^2$ such that $\tilde{x}_2 - \tilde{x}_0^{\delta_2} - \tilde{v}_2^{\delta_1,\delta_2} = \delta_1$ holds (i.e. $\tilde{v}_2^{\delta_1,\delta_2} = \tilde{v}_0 - (\delta_1 + \delta_2)$). For $k = -4$ and $\delta_1 = (-1/5, 1)$, $\delta_2 = (1, -2/5)$ (small perturbation with $(\|\delta_1\|, \|\delta_2\|) = (\sqrt{26/25}, \sqrt{29/25}))$ the data $\tilde{x}_2$, $\tilde{x}_0^{\delta_2} = (-1\frac{2}{5}, -3\frac{3}{5})$ and $\tilde{v}_2^{\delta_1,\delta_2} = (11/5, 17/5)$ satisfy (22). Similarly, for $k = -4$ and $\delta_1 = (-4, 1)$, $\delta_2 = (7, -2)$ (big perturbation with $(\|\delta_1\|, \|\delta_2\|) = (\sqrt{17}, \sqrt{53}))$ the data $\tilde{x}_2$, $\tilde{x}_0^{\delta_2} = (4\frac{3}{5}, -5\frac{1}{5})$ and $\tilde{v}_2^{\delta_1,\delta_2} = (0, 5)$ satisfy (22). Lastly, for $k = -4$ and $\delta_1 = (-12, 1)$, $\delta_2 = (-11, -8)$ (large perturbation with $(\|\delta_1\|, \|\delta_2\|) = (\sqrt{145}, \sqrt{185}))$ the data $\tilde{x}_2$, $\tilde{x}_0^{\delta_2} = (-13\frac{2}{5}, -11\frac{1}{5})$ and $\tilde{v}_2^{\delta_1,\delta_2} = (26, 11)$ satisfy (22). Comparing the graph of $\tilde{\mathcal{E}}_0^d$ from Fig. 1a) with the graphs of $\tilde{\mathcal{E}}_0^\delta$ from Fig. 4 shows that unimodality of $\tilde{\mathcal{E}}_0^d$ is preserved for substantial perturbations $\delta \neq \mathbf{0}$. This trend repeats for other $k \in (k_2, 0) \cup (0, \infty)$ which indicates that in practice the perturbation $\delta = (\delta_1, \delta_2)$ from Proposition 1 can be taken as reasonably large. □

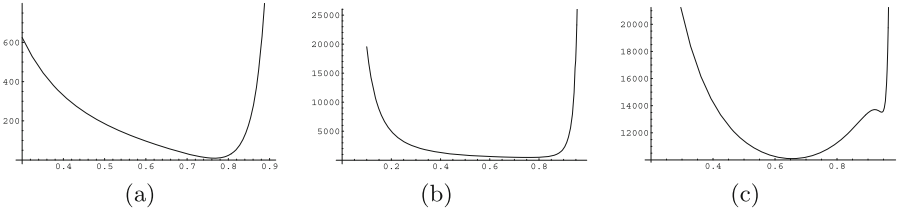(a)   (b)   (c)

Fig. 4. The graph of $\tilde{\mathcal{E}}_0^\delta$ for $k = -4$, $\tilde{x}_0, \tilde{x}_2^{\delta_2}, \tilde{v}_2^{\delta_1,\delta_2} \in \mathbb{R}^2$ and for (a) $\delta_1 = (-1/5, 1)$ and $\delta_2 = (1, -2/5)$ yields a global minimum at $\hat{s}_1(k) \approx 0.76615 \neq \hat{s}_1^{cc}(k) \approx 0.79435$, (b) $\delta_1 = (-4, 1)$ and $\delta_2 = (7, -2)$ yields a global minimum at $\hat{s}_1(k) \approx 0.755816 \neq \hat{s}_1^{cc}(k) \approx 0.874097$, (c) $\delta_1 = (-12, 1)$ and $\delta_2 = (-11, -8)$ yields a global minimum at $\hat{s}_1(k) \approx 0.654924 \neq \hat{s}_1^{cc}(k) \approx 0.945841$, and two other critical points i.e. a local minimum at $\hat{s}_0^1(k) \approx 0.944104$ and a local maximum at $\hat{s}_0^2(k) \approx 0.922$.

6   Conclusions

The optimization task (1) is reformulated into (5) (and (16)) to minimize a highly non-linear multivariate function $\mathcal{J}_0$ depending on knots $\mathcal{T}_{int}$. One of the numerical scheme to handle the latter is *a Leap-Frog*. The *generic case* of this algorithm

is studied in [5]. Here, we complement the latter by analyzing *non-generic case* of *Leap-Frog* and formulate sufficient conditions preserving unimodality of (16). In doing so, first a special case of data (18) is addressed. Subsequently its perturbed analogue (22) is covered. Example shows that unimodality for (18) (if it occurs) is in practice preserved by large perturbations (22). The performance of *Leap-Frog* compared with *Newton's* and *Secant Methods* is reported in [2,3,7]. More applications of *Leap-Frog* are discussed in [10–12]. For related work on fitting (sparse or dense) reduced data $\mathcal{M}_n$ see e.g. [4,6,8].

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