Numerical Analysis.

ON THE SPLINE TRANSFORM OF STEP WISE FUNCTIONS

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ABSTRACT. — We establish some properties of the classical area-preserving spline transform of step wise functions and propose a regularization algorithm for the positive step wise functions whose spline transform fails to be non negative.

KEY WORDS: Histograms, natural cubic splines, spline transform

MATHEMATICS SUBJECT CLASSIFICATION: 41A15, 65D07, 65D10

1. INTRODUCTION

There is a well-known procedure to transform a step-wise function s into a smooth one f when we want to preserve the most important properties of s and, at the same time, operate in an economical way. Let us briefly recall the construction of such smoothing procedure. Unless otherwise specified, all functions are defined on $[a,b]$. Given $N = (x_0, x_1, \dots, x_{n-1}, x_n)$ where $a = x_0 < x_1 < \cdots < x_{n-1} < b = x_n$ and $Q = (q_1, \dots, q_n) \in \mathbb{R}^n$, we denote by $s = [N,Q]$ the step wise function defined by

$$(1)\quad [N,Q](x) = q_i, \quad x \in [x_{i-1}, x_i[, \quad q_i \neq q_{i+1}, \quad i = 1, \dots, n, \qquad \text{and} \quad [N,Q](x_n) = q_n,$$

where the condition $q_i \neq q_{i+1}$ just means that we choose the shortest subdivision. The integer n is called the **length** of $[N,Q]$. When $N = (a,b)$, then $[N,Q]$ is constant equal to q_1, of length one. Histograms correspond to positive step wise functions.

A function $f \in C^1[a,b]$ is said to be an **area-preserving smoothing** for $s = [N,Q]$ as in (1) if the area under f matches that of $[N,Q]$ on the intervals $[x_{i-1}, x_i]$, $i = 1, \dots, n$ where $n = \text{length}([N,Q])$, that is,

$$\int_{x_{i-1}}^{x_i} f(x)\,dx = q_i(x_i - x_{i-1}), \quad i = 1, \dots, n.$$

The particular smoothing f of s that we will study in this paper is the unique area-preserving smoothing of s of minimal L^2 **variation**, that is, minimizing

Date: June 2, 2017.

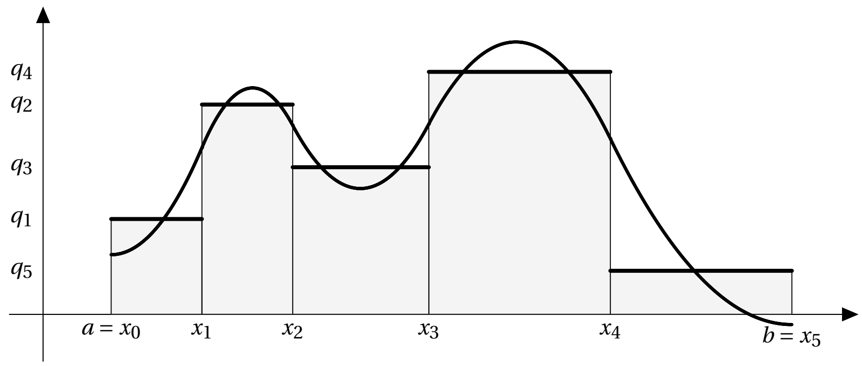


FIGURE 1. A step-wise function $s = [N, Q]$ and its transform $\phi(s)$ with $N = (7.5, 17.5, 27.5, 42.5, 62.5, 82.5)$, $Q = (3.5, 7.7, 5.4, 8.9, 1.6)$ (ratio $y/x = 3$).

the functional $h \mapsto \int_a^b (h'(t))^2 dt$. In fact, see Theorem 1 below, f is the unique area-preserving smoothing for $[N, Q]$ such that :

(CP1) The derivative of f vanishes at the extremities of the interval, that is $f'(a) = f'(b) = 0$.

(CP2) The restriction of f to any of the interval $[x_{i-1}, x_i]$, $i = 1, \dots, n$, is a polynomial of degree at most two.

A common way of computing f is as follows. Setting $V_i = \sum_{j=1}^{i} q_j (x_j - x_{j-1}) = \int_a^{x_i} [N, Q](x) dx$, since f is area-preserving for s, we must have

$$\int_a^{x_i} f(x) dx = V_i, \quad i = 0, \dots, n, \tag{2}$$

where the index $i = 0$ (with $V_0 = 0$) actually adds an empty condition. If F denotes the unique *natural* cubic spline F satisfying $F(x_i) = V_i$, $i = 0, \dots, n$, then we just need to take $f = F'$. Recall that by *natural*, one means that $F''(a) = F''(b) = 0$. In particular, f satisfies properties (CP1) and (CP2) above. We refer to [5, p. 121] for the definition and main properties of natural cubic interpolation splines.

Definition 1. The function f above is called the **spline transform** of $s = [N, Q]$. It will be denoted by $\phi(s) = \phi([N, Q])$ or $\phi(N, Q)$. Its evaluation at $x \in [a, b]$ will denoted by $\phi(N, Q)(x)$ or $\phi(N, Q, x)$.

It is the purpose of this paper to derive some properties, introduce some definitions and raise some problems regarding this transform. The reader may observe the effect of the smoothing procedure in Figure 1. As far as we know, the above definition of the spline transform goes back to [2], but the idea seemed to be in the air at that time, see [4, 8]. A Matlab code for computing the spline transform is available at [1].

Of course, any space of smooth functions on $[a,b]$ in which the interpolation problem (2) has a unique solution provides another natural area-preserving smoothing for s. We may for instance consider other spaces of spline functions. Here, we will just mention the case of polynomials. If P is the unique polynomial of degree at most n such that $P(x_i) = V_i$, $i = 0,\dots,n$, that is, by the Lagrange interpolation formula,

$$P(x) = \sum_{i=0}^{n} V_i \prod_{j=0,\, j\neq i}^{n} \frac{x - x_j}{x_i - x_j}, \tag{3}$$

then $f = P'$ is a polynomial of degree at most $n-1$ that satisfies (2). As indicated above, the main motivation for choosing $\phi(s)$ among all others area-preserving smoothing is the following theorem.

Theorem 1. *The function $\phi(s)$ is the unique area-preserving smoothing for $s = [N,Q]$ with minimal L^2 variation. Thus, setting $\mathcal{V}(f) = \int_a^b (f'(x))^2\,dx$, we have*

$$\mathcal{V}(\phi(s)) = \inf\{\mathcal{V}(f), f \text{ is an area-preserving smoothing for } s\}. \tag{4}$$

The proof is a simple adaptation of the proof of the corresponding variation diminishing property for cubic splines, see [5], and we will omit it.

In section 3, we derive some a-priori estimates on the way the variation $\mathcal{V}(\phi(N,Q))$ depends on N and Q. Such estimates rest on a simple property of spline transforms of length two step wise functions. Some useful observations on the structure of spline transforms are presented in section 2. In practice, apart from the area-preserving property, it is often desirable that the smoothing f respects, in some sense, other elements of the geometry of the graph. For instance, one usually wishes, especially when we have histograms in mind, that the smoothing be non negative. Such property, in general, is not satisfied by the spline transform (as in Figure 1, close to the right extremity of the interval) and this drawback lead to a rich literature where many modifications or alternatives are investigated; the reader may, for instance, consult [3, 6, 7] and the references therein. In this paper, we take a different point of view. The eventual negativity of $\phi(s)$ when s is a positive step wise function is regarded as an exploitable indicator on the structure of s. This is explained in section 4. This point of view seems to lead to natural and interesting questions.

2. Basic properties of the spline transform ϕ

2.1. **Some useful observations.** The following easy properties follow directly from the definition or the characterization properties. Given

$$N = (a, x_1, \dots, x_{n-1}, b),$$

the map $\Phi_N : \mathbb{R}^n \ni Q \longmapsto \phi(N, Q, \cdot) \in C^1([a,b])$ is linear and one-to-one. It is worth observing that $\phi(N, Q+k) = \phi(N, Q) + k$ with $Q + k = (q_1 + k, \dots, q_n + k)$. This is because the right-hand side satisfies the properties (CP1) and (CP2) of $\phi(N, Q+k)$ as well as the area-preserving property. In fact, if $t(x)$ is a polynomial of degree at most two then $\phi(N, Q) + t$ is a spline transform if and only if t is constant (otherwise the conditions on the derivative at the extremities of the interval are not fulfilled).

For $k \in \mathbb{R}$,

$$\phi(N+k, Q, x) = \phi(N, Q, x-k) \quad x \in [a+k, b+k], \tag{5}$$

where $N + k := (a+k, x_1 + k, \dots, x_{n-1} + k, b+k)$ if $N = (a, x_1, \dots, x_{n-1}, b)$. Equivalently, letting τ_k denote the translation $x \to x + k$, $\phi(\tau_k(N), Q) \circ \tau_{-k} = \phi(N, Q)$. There is also an immediate invariance relation with respect to scale transformations. For instance, if $\sigma > 0$ and $h_\sigma[N, Q] := [(\sigma a, \sigma x_1, \dots, \sigma x_{n-1}, \sigma b), Q]$ then

$$\phi(h_\sigma[N, Q])(x) = \phi(N, Q, \sigma^{-1} x), \quad x \in h_\sigma([a,b]). \tag{6}$$

From (5) and (6), we deduce that the map ϕ is invariant under bijective affine maps in a natural sense. In particular, $\phi(s)$ reproduces the standard symmetries that may possess the graph of s.

Lemma 2. *Let $s = [N, Q]$ be a step-wise function of length n on $[a,b]$.*

1. *On the first and on the last interval, $\phi(s)$ is monotone (possibly constant).*
2. *$\phi(s)$ has at most $n-2$ local strict extrema in $]a, b[$.*
3. *We have*

$$\max_{x\in[a,b]} \left| s(x) - \phi(s)(x) \right| \le \max_{1\le i\le n} \sqrt{x_i - x_{i-1}} \sqrt{\int_a^b \Big((\phi(s))'(x) \Big)^2 dx}.$$

Thus, the variation, that is $\mathcal{V}(\phi(N, Q))$, actually controls the uniform approximation of $[N, Q]$ by $\phi(N, Q)$.

Proof. (1) In fact, on both intervals, we have a polynomial of degree at most two whose derivative vanishes at one extremity. Unless it is constant, it cannot vanish somewhere else on one of these intervals.

(2) On each of the $(n-2)$ intervals $[x_i, x_{i+1}]$, $i = 1, \dots, n-2$, $\phi(s)$ is a polynomial of degree at most two and therefore possesses at most one strict local extrema and, according to the previous lemma, there is no strict local extrema in $]a, x_1] \cup [x_{n-1}, b[$.

(3) Write $\phi = \phi(s)$. Let $x \in [x_{i-1}, x_i]$ for $i = 1, \dots, n-1$ (when $i = n$, we may have $x = x_n$). Since

$$\frac{1}{x_i - x_{i-1}} \int_{x_{i-1}}^{x_i} \phi(x)\, dx = q_i,$$

by the mean value theorem, there exists $c \in]x_{i-1}, x_i[$ such that $\phi(c) = q_i$. Hence,

$$\phi(x) - s(x) = \phi(x) - q_i = \phi(x) - \phi(c) = \int_c^x \phi'(x)\,dx. \tag{7}$$

Using Cauchy-Schwarz inequality, we have

$$|\phi(x) - s(x)| \le \int_{x_{i-1}}^{x_i} |\phi'(x)|\,dx \le \sqrt{x_i - x_{i-1}} \sqrt{\int_{x_{i-1}}^{x_i} (\phi'(x))^2 dx}. \tag{8}$$

The claim readily follows. □

2.2. **Reducibility.** We now investigate whether the ϕ-map is one-to-one. To do that, we require the following definitions.

Definition 2. A step-wise function $s = [N, Q]$ is said to be **reducible** if there exists a step-wise function $\hat{s} = [N', Q']$ such that

(1) $\text{length}(\hat{s}) < \text{length}(s)$,
(2) $\phi(\hat{s}) = \phi(s)$.

Non reducible step-wise functions are **irreducible**.

If $\text{length}(\hat{s})$ is minimal among all those $\hat{s}$ such that $\phi(\hat{s}) = \phi(s)$ then $\hat{s} = [N', Q']$ is called a **reduction** for $s = [N, Q]$. The problem of describing the reduction of a given s is readily answered once we introduce the following definition.

Definition 3. The points of $]a, b[$ at which $\phi(s)$ is not twice differentiable are the **nodal points** of $s = [N, Q]$.

The nodal points of s are obviously among the interior entries of N. We will see that, in most cases, they are exactly the interior entries of N. By interior entry of N, we mean the nodes x_i for $0 < i < n$.

Theorem 3. *Every step wise function $s = [N, Q]$ admits one and only one reduction $\hat{s} = [N', Q']$ and the interior entries of N' are exactly the nodal points of s.*

Lemma 4. *If length$(s) > 1$ then $\phi(s)$ is not constant.*

Proof. Indeed, there are at least two different successive values, say q_1 and q_2, see (1), so that

$$q_1 = \frac{1}{x_1 - x_0} \int_{x_0}^{x_1} \phi(s)(x)\,dx \neq q_2 = \frac{1}{x_2 - x_1} \int_{x_1}^{x_2} \phi(s)(x)\,dx,$$

and $\phi(s)$ cannot be constant. □

Proof of Theorem 3. Let $\hat{s} = [N', Q']$ be a reduction of s. If $\text{length}(\hat{s}) = 1$ then $\phi(s) = \phi(\hat{s})$ is constant, and, according to the previous lemma, $\text{length}(s) = 1$, but, in that case, s is irreducible, $\hat{s} = s$ and the assertion of the theorem trivially holds true.

We assume that length$(\hat{s}) = n > 1$ so that $N' = (a, x'_1, \dots, x'_{n-1}, b)$ and we prove that *the points x'_i are nodal points for s.* In fact, if $\phi(s) = \phi(\hat{s})$ was twice differentiable at x'_i, $1 \le i \le n-1$, then the same polynomials of degree at most two would define $\phi(\hat{s})$ on $[x'_{i-1}, x'_i]$ and on $[x'_i, x'_{i+1}]$ (both polynomials would share the same j-th derivative at x'_i for $j = 0, 1, 2$). But, in that case, we could further reduce $\hat{s}$ to $\hat{\hat{s}} = [N'', Q'']$ by removing x'_i from N', that is, taking

$$N'' = (a, x'_1, \dots, x'_{i-1}, x'_{i+1}, \dots, x'_{n-1}, b)$$

and

$$Q'' = \left(q'_1, \dots, q'_{i-1}, \frac{(x_i - x_{i-1}) q'_i + (x_{i+1} - x_i) q'_{i+1}}{x_{i+1} - x_{i-1}}, q'_{i+2}, \dots, q'_n \right),$$

and this would contradict the minimality of the length of $\hat{s}$.

Conversely, since $\phi(\hat{s}) = \phi(s)$, the singular points of the derivative of $\phi(s)$ are singular for the derivative of $\phi(\hat{s})$, the nodal points of $[N, Q]$ must therefore appear in N'. The fact that $\phi(\hat{s})$ is an area-smoothing for s next forces the value for Q', namely if $N' = (a, x_{i_1}, \dots, x_{i_k}, b)$ with $1 \le i_1 < i_2 < \cdots < i_k \le m$ with $m =$ length$([N, Q])$ then

$$q'_k = \frac{\sum_{j=i_k}^{i_{k+1}-1} (x_{j+1} - x_j) q_j}{x_{i_{k+1}} - x_{i_k}}. \qquad \square$$

Example 1. Let $N = (a, x_1, \dots, x_{n-1}, b)$ with $a < x_1 < \cdots < x_{n-1} < b$ and $n \ge 2$. The sets of $Q \in \mathbb{R}^n$ for which $[N, Q]$ is reducible is a union of $n-1$ hyperplanes. In particular it is of empty interior and its Lebesgue measure is null.

Proof. Indeed, to be reducible, there must be at least one of the x_i, $i = 1, \dots, n-1$, which is not a nodal point for $[N, Q]$. But to say that x_i is not nodal means that, say, both constants $\phi''(N, Q)((x_i - x_{i-1})/2))$ and $\phi''(N, Q)((x_{i+1} - x_i)/2))$ coincide. Hence, Q is in the kernel of the linear form

$$\mathbb{R}^n \ni Q \mapsto D^2 \circ \Phi_N((x_i - x_{i-1})/2)) - D^2 \circ \Phi_N((x_{i+1} - x_i)/2)) \in \mathbb{R},$$

which is an hyperplane H_i (D^2 is used for the second derivative and the linear map Φ_N in defined in subsection 2.1. $\square$

Let us denote by **SW** (or **SW**(a, b)) the class of irreducible step wise functions on $[a, b]$ and by $\mathbf{SP}_2$ (or $\mathbf{SP}_2(a, b)$) the class of functions in $C^1([a, b])$ which coincide with a polynomial of degree at most 2 on each interval of a subdivision of $[a, b]$ and with horizontal tangents at the extremities. Clearly, **SW** is the quotient set (that is, is in canonical one-to-one relation with the quotient set) of the equivalence relation $[N, Q] \equiv [M, T]$ if $\phi(N, Q) = \phi(M, T)$. Hence, **SW** is isomorphic to the range of the map $[N, Q] \mapsto \phi(N, Q)$ which is $\mathbf{SP}_2$.

Let us briefly explain how to obtain the pre-image of $f \in \mathbf{SP}_2$. We first select the points (in $]a, b[$) where f is not twice differentiable. This set may be empty (when and only when f is constant) but, by definition of $\mathbf{SP}_2$, it is necessarily finite. We assume that there exists at least one such point and form $N = (x_1, \dots, x_{n-1})$ by correctly ordering them. Next, we set

$$q_i = \frac{1}{x_i - x_{i-1}} \int_{x_{i-1}}^{x_i} f(x)\,dx, \quad i = 1, \dots, n,$$

where $x_0 = a$ and $x_n = b$. We have $\phi(N,Q) = f$.

2.3. **Application.** It seems reasonable to say that a data $[N,Q]$, that is a step wise function $s = [N,Q]$ of length n, in particular a histogram, is ϕ-redundant when $[N,Q]$ is reducible, since a smaller data would return the same spline transform. For computational reasons, exact reducibility, in general, cannot be neither verified nor expected and we should instead introduce a measure of redundancy based on the singular points of the second derivative of the spline transform of $s = [N,Q]$. On $[x_i, x_{i+1}[$, $\phi(s)$ is of the form $a_{i+1}x^2 + b_{i+1}x + c_{i+1}$, the above discontinuity is measured as $|a_{i+2} - a_{i+1}|$.

Definition 4. The **ϕ-redundancy coefficients** g_i and g of $[N,Q]$ are defined as

$$g_i = \frac{|a_{i+2} - a_{i+1}|}{\max_{i=1,\dots,n} |a_i|}, \quad i = 0, \dots, n-2, \quad \text{a}nd \quad g = \min_{i=0,\dots,n-2} g_i.$$

The redundancy coefficient g for the step wise function in Figure 1 is about 0.7 while the coefficient for $(N,Q) = ((1,2,3,4,5),(2,3,6,8))$ is about 0.06, the redundancy arising at $x_3 = 4$.

3. Bounding the variation

To compute a spline transform, following the method sketched in the introduction, we need to solve a cubic spline interpolation problem which amounts to solve a tri-diagonal linear system of order n (or, directly the linear system given below in (19)). This is a reasonably simple computational problem, at least when n is not too big. Yet, one cannot expect a simple closed general expression for $\phi(N,Q)$ and it is therefore interesting to derive a-priori estimates for the variation $\mathcal{V}(\phi(N,Q))$ of a spline transform. To do that, we first concentrate on the simplest cases.

3.1. **Length two case.** When length$([N,Q]) = 1$, $s = [N,Q]$ is constant and equal to its spline transform. Here is a reasonably simple formula when length$(s) = 2$, that is $N = (a, w, b)$ with $a < w < b$. It confirms the intuition that the variation — essentially given by the coefficients of the squared terms — depends on the differences between the q_i and that, keeping it fixed, it grows as w get closer to one of the extremity.

Lemma 5 (Spline transform for length-two step wise functions)**.** *Let $a < w < b$, $N = (a, w, b)$ and $Q = (q_1, q_2)$ the spline transform of $s = [N, Q]$ is given by*

(9)
$$\phi(s)(x) = \left(\frac{q_1(w+2b-3a)+q_2(a-w)}{2(b-a)} + \frac{3(q_2-q_1)(x-a)^2}{2(b-a)(w-a)}\right)\mathrm{charfun}(x,a,w) + \left(\frac{q_1(w-b)+q_2(-w+3b-2a)}{2(b-a)} - \frac{3(q_2-q_1)(x-b)^2}{2(b-a)(b-w)}\right)\mathrm{charfun}(x,w,b),$$

where $\mathrm{charfun}(x,u,v)$ *denotes the characteristic function of the interval* $[u, v[$. *The variation is particularly simple and does not depend on w :*

$$\mathcal{V}\big(\phi(s)\big) = \int_a^b \big((\phi(s))'(x)\big)^2 dx = \frac{3(q_2-q_1)^2}{(b-a)}.$$

Proof. One checks that the right hand side of (9) is an area-preserving smoothing which satisfies the properties (CP1) and (CP2) characterizing $\phi(N,Q)$. The computations are easily done with the help of a computer algebra software. (We used Maxima.) □

Example 2. Step wise functions of length 2 are irreducible.

Proof. In view of Theorem 3, it suffices to show that w is nodal and this follows from a direct computation with (9). □

Observe that (9) shows that $\phi(s)$ is increasing when $q_1 < q_2$ and decreasing when $q_1 > q_2$.

3.2. **Lower bounds.** Lemma 5 enables one to derive simple lower bounds for the variation of any spline transform. In fact, if $s = [N, Q]$ is a step wise function of length n, the restriction of $\phi(s)$ to $[x_{i-1}, x_{i+1}]$ is an area-preserving smoothing for the step wise function $[(x_{i-1}, x_i, x_{i+1}), (q_i, q_{i+1})]$ on the interval $[x_{i-1}, x_{i+1}]$. Its L^2-variation is therefore bigger (or equal) than that of

$$\phi\big((x_{i-1}, x_i, x_{i+1}), (q_i, q_{i+1}), x\big).$$

Hence, in view of Lemma 5,

$$\int_{x_{i-1}}^{x_{i+1}} \big(\phi'(N,Q,x)\big)^2 dx \geq 3\frac{(q_{i+1}-q_i)^2}{x_{i+1}-x_{i-1}}, \tag{10}$$

where, of course, $\phi'(N,Q,x)$ denotes the derivative of $\phi(N,Q)$ with respect to x. More generally, if $0 \leq i < j < k \leq n$, using that $\phi(s)$ is an area smoothing for the step wise function

$$\Big[(x_i, x_j, x_k), \big(\sum_{s=i+1}^{j} q_s(x_{s+1}-x_s), \sum_{s=j+1}^{k} q_s(x_{s+1}-x_s)\big)\Big] \quad \text{on } [x_i, x_k],$$

we obtain the following bound.

Theorem 6. *Let* $[N, Q]$ *be a step wise function of length* n *and* $0 \le i < j < k \le n$. *We have*

$$\int_{x_i}^{x_k} \Big((\phi(s))'(x)\Big)^2 dx \ge 3 \frac{\Big(\sum_{s=i+1}^{j} q_s(x_{s+1}-x_s) - \sum_{s=j+1}^{k} q_s(x_{s+1}-x_s)\Big)^2}{x_k - x_i}. \tag{11}$$

It follows from (10) that

$$\mathcal{V}^2(\phi(s)) \ge 3 \sum_{i=0}^{\lfloor n/2 \rfloor} \frac{(q_{i+2}-q_i)^2}{(x_{i+2}-x_i)}, \tag{12}$$

and a similar lower bound holds for odd indices. More generally, if the right hand side of (11) is denoted by $\mathcal{V}(i, j, k)$ and $0 = i_0 \le i_1 < i_2 < \cdots < i_{2\nu} = n$, using Theorem 6, we have

$$\mathcal{V}^2(f) \ge \mathcal{V}(i_0, i_1, i_2) + \mathcal{V}(i_2, i_3, i_4) + \cdots + \mathcal{V}(i_{2\nu-2}, i_{2\nu-1}, i_{2\nu}).$$

Of course, the best lower bound based on Lemma 5 would be obtained by taking the maximum of the right hand side over all sub-subdivisions of N.

Example 3. From Theorem 6, it follows that if a sequence of step wise functions $[N^d, Q^d]$, $N^d = (x_0^d, \ldots, x_n^d)$, $Q^q = (q_1^d, \ldots, q_n^d)$, is such that, for some $0 < i < j < k$,

$$\frac{1}{x_k^d - x_i^d}\left(\sum_{s=i+1}^{j} q_s^d(x_{s+1}^d - x_s^d) - \sum_{s=j+1}^{k} q_s^d(x_{s+1}^d - x_s^d)\right) \longrightarrow \infty, \qquad d \to \infty,$$

then

$$\lim_{d\to\infty} \mathcal{V}(\phi(N^d, Q^d)) = \infty.$$

In particular, we obtain the intuitively obvious fact that if $\min\{x_{i+1}^d - x_i^d \ : \ i = 0, \ldots, n-1\}$ goes to 0 as d tends to infinity and Q^d remains constant then the variation goes to ∞.

3.3. **Upper bounds.** As for bounding the variation from above, we may use the following observation.

Theorem 7. *Let* $s = [N, Q]$ *be a step wise function of length* n *on* $[a, b]$ *and* $0 \le i < j < k \le n$. *We denote by* $\tilde{s} = [\tilde{N}, \tilde{Q}]$ *the step wise function obtained by deleting the last entries of* N *and* Q. *We have*

$$\mathcal{V}^2(\phi(s)) \le \frac{24(q_n - q_{n-1})^2}{(b - x_{n-1})} + \left(1 + \frac{24(x_{n-1} - x_{n-2})}{(b - x_{n-1})}\right)\mathcal{V}^2(\phi(\tilde{s})). \tag{13}$$

Proof. Let $\phi = \phi(\tilde{s})$ and define f on $[a,b]$ by

$$f(x) = \begin{cases} \phi(x) & (a \le x \le x_{n-1}) \\ \phi(x_{n-1}) + c(x - x_{n-1})^2 & (x_{n-1} \le x \le b) \end{cases},$$

where c is chosen so that

$$\int_{x_{n-1}}^{b} f(x)dx = q_n(b - x_{n-1}). \tag{14}$$

Thanks to the fact that $\phi'(x_{n-1}) = 0$ (the derivative of a spline transform always vanishes at the extremities of its interval which is here $[a, x_{n-1}]$ by definition of $\tilde{s}$), we have that f is C^1 on $[a,b]$, which, together with the definition of c, ensures that f is an area-preserving smoothing for s. It follows that

$$\mathcal{V}^2(\phi(s)) \le \mathcal{V}^2(f) = \mathcal{V}^2(\phi(\tilde{s})) + \int_{x_{n-1}}^{b} (f'(x))^2 dx. \tag{15}$$

Now, we have

$$\int_{x_{n-1}}^{b} (f'(x))^2 dx = \frac{4c^2}{3}(b - x_{n-1})^3, \tag{16}$$

and, from (14) one readily checks that $c = \frac{3}{(b-x_{n-1})^2}\big(q_n - \phi(x_{n-1})\big)$, so that

$$\int_{x_{n-1}}^{b} (f'(x))^2 dx = \frac{12}{(b - x_{n-1})}\big(q_n - \phi(x_{n-1})\big)^2, \tag{17}$$

and, using the inequality $(\alpha + \beta)^2 \le 2(\alpha^2 + \beta^2)$,

$$\int_{x_{n-1}}^{b} (f'(x))^2 dx \le \frac{24}{(b - x_{n-1})}\big((q_{n-1} - \phi(x_{n-1}))^2 + (q_n - q_{n-1})^2\big). \tag{18}$$

Now, since $q_{n-1} = \tilde{s}(x_{n-1})$, a use of inequality (8) in the proof of Lemma 2 yields

$$(q_{n-1} - \phi(x_{n-1}))^2 \le (x_{n-1} - x_{n-2})\mathcal{V}^2(\phi(\tilde{s})).$$

Thus, in view of (18), we have

$$\int_{x_{n-1}}^{b} (f'(x))^2 dx = \frac{24}{(b - x_{n-1})}\left\{(q_n - q_{n-1})^2 + (x_{n-1} - x_{n-2})\mathcal{V}(\phi\big(\tilde{N}, \tilde{Q})\big)\right\},$$

and, turning to (15), we arrive at (13). □

We may now use repeatedly the above theorem as follows. Setting

$$\Delta q_i := \frac{(q_i - q_{i-1})^2}{x_i - x_{i-1}} \quad \text{and} \quad \Delta x_i := \frac{x_{i-1} - x_{i-2}}{x_i - x_{i-1}},$$

we have

$$\mathcal{V}^2(\phi(N,Q)) \le \sum_{i=0}^{n-4} 24\Delta q_{n-j} \prod_{j<i}(1+24\Delta x_{n-j}) + \mathcal{V}^2\Big(\phi\big((x_0,x_1,x_2),(q_1,q_2)\big)\Big) \prod_{j<n-3}(1+24\Delta x_{n-j}),$$

hence, in view of Lemma 5,

$$\mathcal{V}^2\Big(\phi(N,Q)\Big) \le \sum_{i=0}^{n-4} 24\Delta q_{n-j} \prod_{j<i}(1+24\Delta x_{n-j}) + \frac{3(q_2-q_1)^2}{(a-x_2)} \prod_{j<n-3}(1+24\Delta x_{n-j}),$$

where, as usual, an empty product is taken to be one.

Example 4. If $[N^d,Q]$ is a sequence of stepwise functions of length n (Q fixed) — such that $\min_{0\le i\le n-1}(x^d_{i+1}-x^d_i)$ tends to 0 as $d\to\infty$ but $\max_{2\le i\le n}\Delta x^d_i$ remains bounded — then $\mathcal{V}(\phi(N^d,Q))$ tends to 0 as $d\to\infty$.

We mention still another way of obtaining elementary upper bounds. Let $s=[N,Q]$ be a stepwise function of length n as above. For $1<i<n-1$, we write $N_i=(a,x_1,\dots,x_{i-2},x_{i-1})$, $Q_i=(q_1,\dots,q_{i-1})$, $N^i=(x_i,x_{i+1},\dots,x_{n-1},b)$, $Q^i=(q_{i+1},\dots,q_n)$, $\phi_i=\phi(N_i,Q_i)$ and $\phi^i=\phi(N^i,Q^i)$ then we have

$$\mathcal{V}^2\Big(\phi(N,Q\mid a,b)\Big) \le \mathcal{V}^2(\phi_i)+\mathcal{V}^2(p)+\mathcal{V}^2(\phi^i)$$

where p is the unique polynomial of degree 4 which is tangent to ϕ_i at x_{i-1}, to ϕ^i at x_i and such that $\int_{x_{i-1}}^{x_i} p(x)dx = q_i(x_i-x_{i-1})$. (The existence and uniqueness of such polynomial is easily shown). Again, the estimate follows from the fact that the function obtained on suitably glueing ϕ_i, p and ϕ^i is a preserving-area smoothing for $[N,Q]$, so that its variation is not smaller than that of $\phi(N,Q)$.

4. Regularity and regularization

As explained in the introduction, it is often desirable that the smoothing $\phi=\phi(s)$ of a (strictly) positive step wise function $s=[N,Q]$ be not negative and this property is not guaranteed by the spline transform, see the example in Figure 1 (close to the right extremity). This may be interpreted in two different ways. We may consider that the spline transform is not, at least in these cases, a suitable smoothing procedure and may therefore look for other techniques. One might for instance look for splines minimizing more involved kernels than the plain $f\to\int_a^b (f'(t))^2dt$ used here, or one might try to use other types of approximants. We refer to the references indicated in the introduction for more on these approaches. Here, we look at the eventual negativity of $\phi(s)$, not as a defect of the spline transform, but as an indicator that the definition of s is defective, that is, that the subdivision N is not well adapted to the data Q. We provide an algorithm which gives a plausible redistribution (refining the original one) of the data $[N,Q]$.

Let us point out that, when s is obtained, for instance, from experimental data or from a practical problem, the pertinence of the redistribution provided by our algorithm must be analysed in light of the experiment which produced the data.

4.1. **Singularities.** We define the three forms of negativity that a spline transform may exhibit, each of them leading to a different kind of singularity which will be handled in a different way.

Definition 5. A (strictly) positive step wise function $[N,Q]$ on $[a,b]$ is said to be **regular** or **ϕ-regular** when its spline transform is positive (or null) on $[a,b]$. Non regular step wise functions are singular.

We will distinguish three types of singularities. Let $s = [N,Q]$ be a strictly positive step wise function of length n and $\phi = \phi(N,Q)$ its spline transform.

(LS) s has a **left singularity** when $\phi(a) < 0$.
Thus, by continuity, there exists $\epsilon > 0$ such that $\phi < 0$ on $[a, a+\epsilon[$. Since $\int_a^{x-1} \phi(x)dx = q_1 > 0$, we necessarily have $\epsilon < a - x_1$.

(RS) Likewise, s has a **right singularity** when $\phi(b) < 0$.
There exists $\epsilon > 0$ such that $\phi < 0$ on $[b-\epsilon, b]$. As above, we necessarily have $\epsilon < b - x_{n-1}$.

(IS) s has an **interior singularity** when ϕ has a (strictly) negative relative minima in $]a,b[$.
In fact, since, see Lemma 2, ϕ is monotone on the $[a,x_1]$ and on $[x_{n-1},b]$, such a minima can only appear in $[x_1,x_{n-1}]$. Thus, in presence of an interior singularity, on some $]c,d[$ with $a < c$ and $d < b$ and, for some $\epsilon > 0$ $\phi \geq 0$ on $[c-\epsilon, c] \cup [d, d+\epsilon[$. Such subinterval $|c,d[$ cannot contain the whole of an interval $]x_i, x_{i+1}[$.

For instance, the step wise function in Figure 1, which we will regularize below (Fig. 2 (B)), has a right singularity and the step wise function in Figure 2 (B)) has one interior singularity and a right singularity. Typically, interior singularities appear when small values of q_i alternate with big ones.

Lemma 8.

1. *All step-wise functions of length* 1 *are regular.*
2. *Step-wise functions of length* 2 *may have only one (left or right) singularity.*
3. *A step-wise function of length* 3 *cannot have both an interior singularity and a left (or right) singularity.*

Proof. The claim is obvious in the case of length 1. The second claim follows from the fact that if s is of length two then $\phi(s)$ is either increasing when $q_1 < q_2$ or decreasing when $q_2 < q_1$, see Lemma 5. Now, assume that s is of length 3 and has an interior singularity. It has a strict local (negative) minimum, say at c and, according to Lemma 2, no other strict extrema in $]a,b[$. Since $\phi(c) < 0$, ϕ is decreasing on $]a,c[$ and increasing on $]c,a[$ and therefore possesses no left or right singularity. □

4.2. **Dealing with singularities.** We will describe a regularization procedure that enables to obtain a positive functions starting from singular step wise functions. Let us first concentrate on the simplest case of length two step wise functions. Suppose that $s = [(a,w,b),(q_1,q_2)]$ with $q_2 < q_1$ has a right singularity so that, writing $\phi = \phi(s)$ and using (9), we have

$$\phi(b) = \frac{-q_1(b-w) + q_2(-w+3b-2a)}{2(b-a)} < 0 \implies q_2 < q_1 \frac{b-w}{3b-w-2a}.$$

In particular, since, $3b-w-2a > 3(b-w)$, we must have $3q_2 < q_1$. We set $b(u) = w + u(b-w)$ and $q_2(u) = q_2/u$ so that for $u \in]0,1]$, $q_2(b-w) = q_2(u)(b(u)-w)$. The function $f :]0,1] \ni u \mapsto \phi(b(u))$ satisfies $f(1) = \phi(b) < 0$ by hypothesis and a simple calculation shows that $3(b(u)-a)f(u) = q_1(w-a) > 0$. Hence f vanishes for some $u^\star$ between $3q_2/2q_1$ and 1 so that the step wise function

$$[(a,w,b(u^\star)),(q_1,q_2(u^\star))]$$

is regular (with rectangles of same area as $[(a,w,b),(q_1,q_2)]$). This provides a regularization for $[(a,w,b),(q_1,q_2)]$.

More generally, the following lemma is useful to deal with right singularities. Of course, a similar result holds for left singularities because

$$[(x_0,\ldots,x_n),(q_1,\ldots,q_n)]$$

has a left singularity if and only if

$$[(-x_n,\ldots,-x_0),(q_n,\ldots,q_0)]$$

has a right singularity. .

Lemma 9. *Let $[N,Q]$ be a strictly positive step wise function of length n on $[a,b]$. We denote by ϕ its spline transform. If*

(1) $\phi(x_{n-1}) > 0$, $\phi(x_{n-2}) > 0$,
(2) $2q_n \geq 3q_{n-1} > 0$,

then ϕ is increasing (or constant) on the interval $[x_{n-1},b]$.

Since, $\phi(x_{n-1}) > 0$, it follows that ϕ is positive on $[x_{n-1},b]$.

Proof. Let $r = \phi(x_{n-1})$ and $s = \phi'(x_{n-1})$. Recall that by Lemma 2, ϕ is monotone on $[x_{n-1}, b]$. It suffices to show that $r \le q_n$. Indeed, if this occurs, ϕ must be increasing or constant as claimed for, otherwise, the area-preserving condition on $[x_{n-1}, x_n]$ could not be satisfied. We prove that the reverse inequality $r > q_n$ leads to a contradiction. In fact, the inequality $r > q_n$ together with Lemma 2 implies that ϕ is decreasing (not constant) on $[x_{n-1}, b]$, hence $s < 0$. This means that ϕ is decreasing on some interval $[c, x_{n-1}]$ and, since $q_{n-1} < q_n$ (see assumption 2), in order to satisfy the area-preserving condition, it must be increasing on $[x_{n-2}, c]$, where $x_{n-2} < c < x_{n-1}$. Hence ϕ is concave on $[x_{n-2}, x_{n-1}]$. On this interval, it is of the form

$$\phi(x) = r + s(x - x_{n-1}) + \gamma(x - x_{n-1})^2,$$

and

$$\min\{\phi(x)\, x \in [x_{n-2}, x_{n-1}]\} = \min\{\phi(x_{n-2}), \phi(x_{n-1})\} = \phi(x_{n-2}),$$

the last equality because of the area-preserving condition on $[x_{n-2}, x_{n-1}]$ and the fact that $q_{n-1} < q_n$. In fact, the area-preserving condition on $[x_{n-2}, x_{n-1}]$ readily yields an expression for γ in terms of r and s,

$$\gamma = \frac{3(x_{n-1} - x_n)s + 6(q_{n-1} - r)}{2(x_{n-1} - x_{n-2})^2}.$$

This equation in turn gives

$$\phi(x_{n-2}) = (x_{n-1} - x_{n-2})s/2 + (3q_{n-1} - 2r).$$

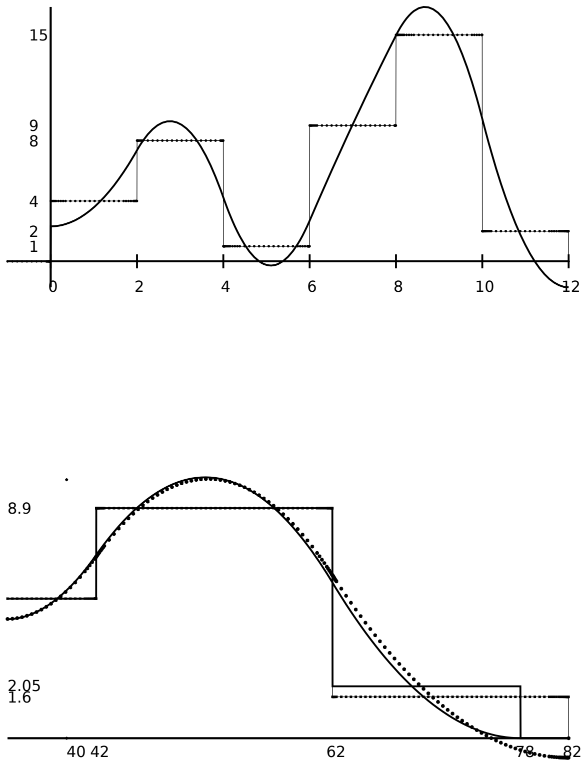
Since $s < 0$, the positivity of $\phi(x_{n-2})$, see assumption (1), implies $3q_{n-1} - 2r > 0$ or $3q_{n-1} > 2r$ and since $r \ge q_n$ this gives $3q_{n-1} > 2q_n$ which is contrary to the assumption. □

For instance, in Figure 1, we took $q_5 = 1.6$ and $q_4 = 8.9$ so that the second assumption is not satisfied and, in fact, $\phi(N, Q)$ is not positive on the last interval while it is positive on the previous one.

Lemma 10. *Let $N_\beta = (a, x_1, \dots, x_{n-1}, \beta)$ with $x_{n-1} < \beta \le b$,*

$$Q_\beta = (q_1, \dots, q_{n-1}, q_n \frac{b - x_{n-1}}{\beta - x_{n-1}}),$$

and $s_\beta = [N_\beta, Q_\beta]$. We denote by ϕ_β the spline transform of s_β. The function $\beta \to \phi_\beta(\beta)$ is continuous on $]x_{n-1}, b]$.



(A) The step-wise function $s = [N, Q]$ with $N = (0, 2, 4, 6, 8, 10, 12)$ and $Q = (4, 8, 1, 9, 15, 2)$ and its spline transform.

(B) The function $\phi(s)$ in Figure 1, near the right extremity, together with a regularization $\phi(\tilde{s}), \tilde{s} = [\tilde{N}, \tilde{Q}]$ with $\tilde{N} = (7.5, 17.5, 27.5, 42.5, 62.5, 78.43)$, and $\tilde{Q} = (3.5, 7.7, 5.4, 8.9, 2)$.

FIGURE 2. Examples of singular and regularized step-wise functions.

Proof. The function ϕ_β can be written as $\phi_\beta(x) = c_0 + c_1 x + c_2 x^2 + \sum_{j=1}^{n-1} c_{j=2}(x - x_j)_+^2$ where the $(n+2)$ coefficients c_j are given by the conditions

$$\phi'_\beta(x_0) = 0, \int\limits_{x_{i-1}}^{x_i} \phi_\beta(x)\,dx = q_i(x_i - x_{i-1}), 1 \le i \le n-1, \tag{19}$$

$$\int\limits_{x_{n-1}}^{\beta} \phi_\beta(x)\,dx = q_n(b - x_n),\ \phi'_\beta(\beta) = 0.$$

To prove the claim, it suffices to show that $C = (c_0, \dots, c_{n+1})$ depends continuously on β where C is the solution of the linear system $AB = C$ corresponding to (19). Observe that B does not depend on β. So, it suffices to show that the coefficients of A (which is invertible for every $\beta \in]x_{n-1}, b]$) depend continuously on β. Only the last two lines of A (the conditions being ordered as in (19)) depend on β,

$$A = \begin{pmatrix} * & * & * & * & \dots & * \\ (\beta - x_{n-1}) & \frac{\beta^2 - x_{n-1}^2}{2} & \frac{\beta^3 - x_{n-1}^3}{3} & \frac{(\beta - x_2)^3 - (x_{n-1} - x_1)^3}{3} & \dots & \frac{(\beta - x_{n-1})^3}{3} \\ 0 & c_1 & 2\beta & 2(\beta - x_2) & \dots & 2(\beta - x_{n-1}) \end{pmatrix},$$

and the continuity follows. □

4.3. **A regularization algorithm.** Let $s = [N, Q]$ be a step wise function of length n and $\phi = \phi(s)$. We present an algorithm which, when ϕ is singular, returns a sum of non negative spline transforms of certain natural re-arrangements of s, obtained by replacing the value of s by zero on certain subintervals, while keeping the same area on each original interval. Such function is itself area-preserving for the initial s but it is not, in general, smooth (see however the comments below). Two different regularizations of a singular step wise function are drawn in Figure 4.

The general strategy is as follows.

In the case of an interior singularity, say on $[x_j, x_{j+1}]$, we separate $[N, Q]$ in two distinct step wise functions $[N_1, Q_1]$ and $[N_2, Q_2]$, the first one on $[a, a']$ and the second one on $[a', b]$ with $x_j < a' < x_{j+1}$ and

$$N_1 = (a, x_1, \dots, x_j, a'), \quad Q_1 = (q_1, \dots, q_{j-1}, q'), \quad \text{and}$$
$$N_2 = (a', x_{j+1}, \dots, x_{n-1}, b), \quad Q_2 = (q'', q_{j+1}, \dots, q_n),$$

where

$$q'(a' - x_j) + q''(x_{j+1} - a') = q_j(x_{j+1} - x_j).$$

The case where a' is one of the entries of N is easily treated, see Line 6 in Algorithm 1. In case of multiple interior singularities, Algorithm 1 starts with the deepest negative value. Another reasonable choice would be to cut where the negative area is maximal. We might also decide to cut at its centre the interval containing the worst (in one of the above senses) singularity.

As for the values of q' and q'', we may for instance divide the area of the rectangle of base $[x_i, x_{i-1}]$ into the two new rectangles of base $[x_j, a']$ and $[a', x_{j+1}]$ proportionally to the length of the new rectangles, that is $q' = q_{j+1}$ and $q'' = q_{j+1}$. This is the strategy implemented in Algorithm 1. Another one would be to allocate half of the area independently from the length of the bases. In general, such cutting transforms an interior singularity into a right singularity for

Data: $[N,Q]$
Result: A regularization of the spline transform of $[N,Q]$
Initialization : $S=\{[N,Q]\}$, test $=\#\mathrm{sing}([N,Q])$, choose $\epsilon>0$;
while test >0 **do**
  for $s=\left[(s_1^1,\dots,s_n^1),(s_1^2,\dots,s_{n-1}^2)\right]\in S$ **do**
    Remove s from S;
    if *s has a interior singularity* **then**
      Choose a among the interior singularity of $\phi(s)$ with **smallest value**;
      if *a is a point in s_1, say $a=s_i^1$,* **then**
        $s':\left[(s_1^1,\dots,s_i^1),(s_1^2,\dots,s_{i-1}^2)\right]$; $s'':\left[(s_i^1,\dots,s_n^1),(s_i^2,\dots,s_{n-1}^2)\right]$;
        Adjoin s' and s'' to S.
      end
      else
        Select i such that $a\in]s_i^1,s_{i+1}^1[$;
        $q_1=s_i^2\cdot(s_{i+1}^1-s_i^1)/(a-s_i^1)$, $q_2=s_i^2\cdot(s_{i+1}^1-s_i^1)/(s_{i+1}^1-a)$;
        $s':\left[(s_1^1,\dots,s_i^1,a),(s_1^2,\dots,s_{i-1}^2,q_1)\right]$, $s'':\left[(a,s_i^1,\dots,s_n^1),(q_2,s_i^2,\dots,s_{n-1}^2)\right]$;
        Adjoin s' and s'' to S.
      end
      test = test + $\#\mathrm{sing}(s')+\#\mathrm{sing}(s'')-\#\mathrm{sing}(s)$
    end
    else if *s has a right singularity* **then**
      $s'=s$;
      repeat
        ${s'}_n^1={s'}_n^1-\epsilon(s_n^1-s_{n-1}^1)$, ${s'}_{n-1}^2=s_{n-1}^2\cdot(s_n^1-s_{n-1}^1)/({s'}_n^1-s_{n-1}^1)$
      until *s' has no right singularity or has an interior singularity*;
      Adjoin s' to S;
      test = test + $\#\mathrm{sing}(s')-\#\mathrm{sing}(s)$
    end
    else if *s has a left singularity* **then**
      $s'=s$;
      repeat
        ${s'}_1^1={s'}_1^1+\epsilon(s_2^1-s_1^1)$, ${s'}_1^2=s_1^2\cdot(s_2^1-s_1^1)/(s_2^1-{s'}_1^1)$
      until *s' has no left singularity or has an interior singularity*;
      Adjoin s' to S;
      test = test + $\#\mathrm{sing}(s')-\#\mathrm{sing}(s)$
    end
  end
end
return $R\phi([N,Q])(x)=\sum_{s\in S}\phi(s)\cdot\mathrm{charfun}(x,s_1^1,s_{\mathrm{last}}^1)$

FIGURE 3. Regularization algorithm

$[N_1,Q_1]$ and a left singularity for $[N_2,Q_2]$. It may happens, however, that there remains only one left (or right) singularity after cutting.

Table 1 summarizes a few natural cutting strategies. We assume as above that a negative minima is reached at $a' \in]x_j, x_{j+1}[$. To deal with singularities

	Old $N \to$ New N_1,N_2	Old $Q \to$ New Q_1,Q_2
P: Proportional	$N_1=(x_0,\dots,x_j,a')$, $N_2=(a',x_{j+1},\dots,x_n)$	$Q_1=(q_1,\dots,q_j,q_{j+1})$, $Q_2=(q_{j+1},\dots,q_{n-1},q_n)$
ON: Optimized for Negativity	$N_1=(x_0,\dots,x_j,a')$, $N_2=(a',x_{j+1},\dots,x_n)$	$Q_1=(q_1,\dots,q_j,\alpha')$, $Q_2=(\alpha'',\dots,q_{n-1},q_n)$ where $\alpha'=\alpha q_{j+1}\frac{x_{j+1}-x_j}{a'-x_j}$ and $\alpha''=(1-\alpha)q_{j+1}\frac{x_{j+1}-x_j}{x_{j+1}-a'}$ where $\alpha \in]0,1[$ is chosen to ensure negativity of both spline transforms at a'.
PC: Proportional at Center	$N_1=(x_0,\dots,x_j,m_j)$, $N_2=(m_j,x_{j+1},\dots,x_n)$ with $m_j=(x_j+x_{j+1})/2$.	$Q_1=(q_1,\dots,q_j,q_{j+1})$, $Q_2=(q_{j+1},\dots,q_{n-1},q_n)$
OV: Overlapping	$N_1=(x_0,\dots,x_j,x_{j+1})$, $N_2=(x_j,x_{j+1},\dots,x_n)$	$Q_1=(q_1,\dots,q_j,q_{j+1}/2)$, $Q_2=(q_{j+1}/2,\dots,q_{n-1},q_n)$

TABLE 1. Some cutting strategies

at an extremity, we use length reduction of the interval. For instance, in the case of a right singularity at $b=x_n$, starting from $N=(x_0,\dots,x_n)$ and $Q=(q_1,\dots,q_{n-1},q_n)$, we set

(20) $$N'=(x_0,\dots,x_{n-1},x_n-\epsilon) \quad \text{and} \quad Q'=(q_1,\dots,q_{n-1},q_n\frac{x_{n-1}-x_n}{x_{n-1}-x_n-\epsilon}),$$

so that

(21)
$$q_n(x_n-x_{n-1})=\int_{x_{n-1}}^{x_n}\phi(N,Q)(x)dx=\int_{x_{n-1}}^{x_n-\epsilon}\phi(N',Q')(x)=q'_n(x_n-\epsilon-x_{n-1}).$$

Lemma 9 shows that a sufficient reduction will provide positiveness. However, it does not rule out (though it seems to be unlikely) that the process of reduction brings about a new interior singularity and the algorithm takes this point into account. The algorithm uses a rude reduction step ϵ. In practice, we took ϵ as 0.5 percent of the length of the original interval. In an optimized algorithm, it is advisable to adapt ϵ to the level of negativity encountered and (or) to refine a rough positive value using a bisection algorithm (based on Lemma 10). In fact, by suitably adapting the algorithm, when starting with a negative value, it produces a solution which is actually null at the (moving) extremity of the reduced interval (the "‘first"’ available solution when performing a reduction). The existence of such exact value follows from the continuity of the function $b \mapsto \phi_b(b)$ proved in Lemma 10. The cutting strategy **ON**, see Table 1, is intended for the computation of such type of regularization.

The algorithm obviously terminates since $\phi(s)$ has a finite number of negative minima. Any regularization algorithm based on a cutting strategy (not necessarily of one the type made explicit in Table 1 coupled with a length reduction process will be called a **cutting-reduction algorithm**. Our algorithm (and any of its variants) returns a sum of spline transforms of step wise functions of smaller lengths and disjoint supports. Because of the reduction process, when the function does not coincide with its regularization, it is (a priori) defined on a strict subset X of $[a,b]$. We may extend it as 0 on $[a,b]\setminus X$ (as in done in Figure 4) and denote by $\mathscr{R}\phi(s)$. Note that, in general, $\mathscr{R}\phi(s)$ is discontinuous at each junction point. Thus, we have a relation of the form

$$\mathscr{R}\phi(s)(x) = \sum_{j=1}^{k} \phi(s_k)(x) \quad \text{for } x \text{ in the support of } \mathscr{R}\phi(s), \tag{22}$$

where the $\phi(s_k)$ have disjoint supports. For instance, in the case of the **P** regularization in Figure 4 for $s = [N,Q]$, $N = (0,2,4,6,8,10,12)$ and $Q = (4,8,1,9,15,2)$, up to computational errors, we have $k = 3$ and

$$\begin{aligned}
s_1 &= [(1.2799,3,7,7.3421),(1.744,8,0.4569)],\\
s_2 &= [(7.6438,8,10,14,15.339),(0.4034,7,12,1.6217)],\\
s_3 &= [(16.1714,17,23),(1,5)].
\end{aligned}$$

Observe that the **ON** regularization in Figure 4 looks like a smooth function on the whole of $[a,b]$ but it is not even continuous. In general, our algorithm will not provide a smooth regularization on $[a,b]$. The reason is that when both a left and a right singularity are to be removed, there are treated separately. For instance, when regularizing s in Figure 4, we cut s near 7, say at a' and near 16, say at b' so that at the next step we need to regularize $s' = [N',Q']$ with $N' = (a',8,10,14,b')$ with a right singularity at b' and a left singularity at a'. Algorithm 1 will first deal with b' and provide a modification $s'' = [N'',Q'']$ of s' whose spline transform may be taken to be 0 at the last point b'' of N'', hence $\phi(s'') = 0$ and $\phi'(s'') = 0$ so that $\phi(s'')$ is smoothly extended to 0 on $[b'',b']$. Next we need to treat the left singularity at a' and, this will change, even if very slightly, the value at b'', thus breaking the smoothness previously obtained. Clearly, in order to preserve smoothness, we should deal simultaneously with both singularities and this raises the following question.

Question 1. Can we always simultaneously remove both a left and a right singularity by performing (non identical) simultaneous left and right reductions?

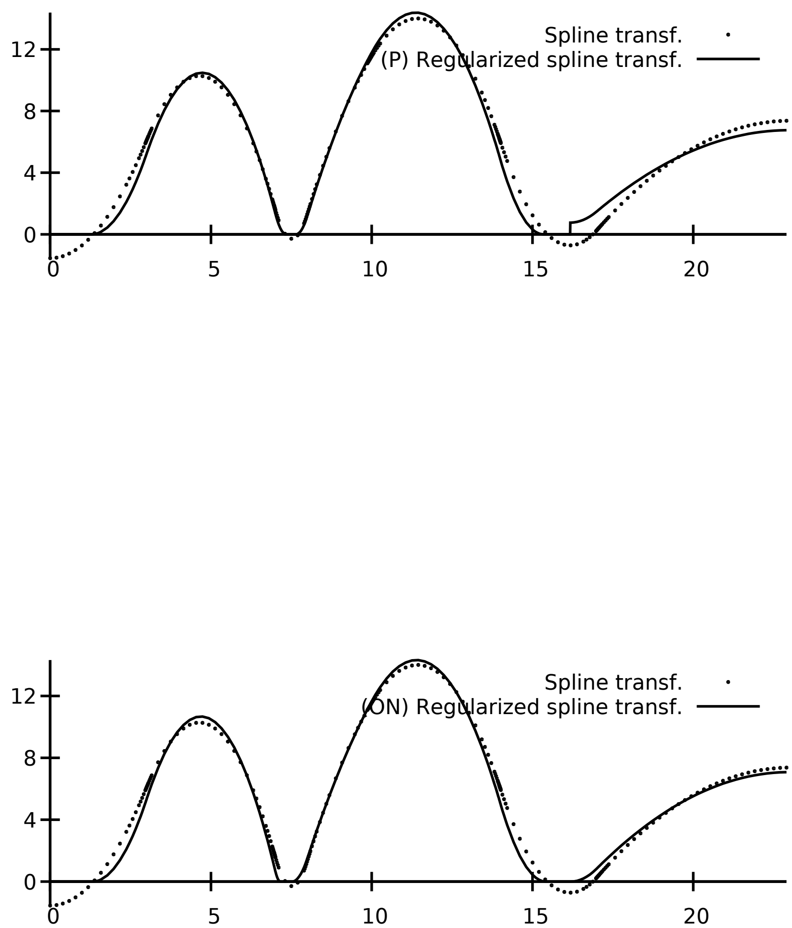


FIGURE 4. An example of spline and regularized spline transforms for $s = [N, Q]$, $N = (0, 2, 4, 6, 8, 10, 12)$ and $Q = (4, 8, 1, 9, 15, 2)$.

Yet, **ON** regularization may be considered as an acceptable approximation of a smooth regularization that may suffice in applications. In any case, in the example above, the sum of the jumps at discontinuities is clearly smaller that that provided by the **P** regularization. The various natural available strategies lead to the following questions.

Question 2. Is there a cutting-reduction algorithm that minimizes the sum of the jumps at the discontinuities of $\mathscr{R}\phi(s)$ for a given s?

Question 3. Is there a cutting-reduction algorithm that minimizes the sum of the variation of the spline transforms forming $\mathscr{R}\phi(s)$ for a given s?

Acknowledgement. We thank an anonymous referee for a careful reading of the manuscript.

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