General Spline Filters for Discontinuous Galerkin Solutions

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Abstract

The discontinuous Galerkin (dG) method outputs a sequence of polynomial pieces. Post-processing the sequence by Smoothness-Increasing Accuracy-Conserving (SIAC) convolution not only increases the smoothness of the sequence but can also improve its accuracy and yield superconvergence. SIAC convolution is considered optimal if the SIAC kernels, in the form of a linear combination of B-splines of degree d, reproduce polynomials of degree $2d$. This paper derives simple formulas for computing the optimal SIAC spline coefficients for the general case including non-uniform knots.

1 Introduction

The Discontinuous Galerkin (dG) method is widely used to approximately solve the weak formulation of partial differential equations. The lack of continuity between the dG elements models weak constraints between elements and is computationally convenient: discontinuity allows for a flexible discretization of the partial differential equations by locally adjusting the polynomial degree and element spacing; and the discontinuity increases opportunities for parallelism when stepping forward in a simulation. However, except near jump discontinuities, the inter-element discontinuities often do not agree with the expected smoothness of the outcome and hinders downstream applications such as stream line tracing [WRKH09].

Filtering, in particular Smoothness-Increasing Accuracy-Conserving (SIAC) filtering, has been proposed to smooth dG output while maintaining the order of the accuracy of the original dG solution. Remarkably, such post-filtering by convolution, can improve the accuracy of the resulting approximation as a solution to the partial differential equations, not only for dG, but also for other Galerkin-projection methods. Already Bramble and Schatz [BS77] showed that, for a wide class of elliptic boundary value problems and uniform subdivision of the domain, averaging of the output can yield superconvergence, i.e. a more accurate approximation to the solution than the degree of the elements suggests. Superconvergence is possible since certain integral norms, called moment norms [ML78] or negative-order norms, converge fast and this can be used to bound the error of the convolved output. In the context of linear hyperbolic partial differential equations this fact was convincingly demonstrated in [CLSS03].

Starting with [CKRS07], a series of papers has generalized SIAC filtering of dG output from the prototypical case of linear equations with periodic boundary conditions on a uniform mesh to non-uniform meshes and spatial dimensions two and three, including structured and unstructured bivariate and tetrahedral meshes [MJRK11, MKRK13, MRK14]. A recent advance, presented in the minisymposium on post-processing dG solutions [MR14] organized by Mirzargar and Ryan, are simple formulas that allow solving for the coefficients of optimal SIAC spline filters with uniform knots. By contrast, [MRK12] had to resort to Gaussian quadrature to determine the entries of the corresponding constraint matrix. Since the SIAC approach itself has recently been extended to non-uniform meshes, formulas corresponding to B-splines with non-uniform knot spacing deserve attention. This paper is first to derive the formulas for this case, and prove uniqueness.

Overview Section 2 reviews, to the extent needed for the results, B-splines, SIAC filtering and convolution. Section 3 derives the entries of the constraint matrix whose solution yields the optimal coefficients for filters that post-process dG solutions with splines over non-uniform knot sequences. Section 4 discusses special choices of knot sequences.

2 Convolution and B-splines

The goal of SIAC filtering is to smooth out the sequence of polynomial pieces p_j, $j = 0..n$ on consecutive intervals $[t_j..t_{j+1}) \subsetneq \mathbb{R}$ that are output by dG computations. To this end, we will convolve the sequence with a linear combination of

B-splines. The convolution $f * g$ of a function f with a function g is defined as

$$(f * g)(x) := \int_{\mathbb{R}} f(t)g(x-t)dt = (g * f)(x), \tag{1}$$

for every x where the integral exists. When $g \geq 0$ and $\int_{\mathbb{R}} g = 1$ then the convolution has special, desirable properties: if f is non-negative, (directionally) monotone or if f is convex then so is $f * g$. Moreover, the graph of $f * g$ is in the convex hull of the graph of f. Convolution is commutative, associative and distributive.

A succinct but comprehensive treatment of B-splines can be found in Carl de Boor's summary [dB02] (see also [Sch81]). There are a number of alternative ways to derive and define B-splines, for example as the smoothest class of piecewise polynomials over a given support. The subclass of uniform B-splines can alternatively be defined via convolution (efficiently carried out in Fourier space), a definition that is handy when deriving optimal coefficients of SIAC spline filters with *uniform* knot spacing. For general, non-uniform filters, the classical definition of splines via divided differences [CS66] is more convenient. We use the notation $i : j$ to abbreviate the sequence $i, i+1, \ldots, j-1, j$ and $t_{i:j}$ correspondingly to denote the sequence of real numbers $t_i, t_{i+1}, \ldots, t_j$. For a sufficiently smooth univariate real-valued function h with kth derivative $h^{(k)}$, divided differences are defined by[1]

$$\begin{aligned}
&\Delta(t_i)h := h(t_i), && \text{and for } j > i \\
&\Delta(t_{i:j})h := \begin{cases} (\Delta(t_{i+1:j})h - \Delta(t_{i:j-1})h)/(t_j - t_i), & \text{if } t_i \neq t_j, \\ \frac{h^{(j-i)}}{(j-i)!}(t_i), & \text{if } t_i = t_j. \end{cases}
\end{aligned} \tag{2}$$

If $t_{i:j}$ is a non-decreasing sequence, we call its elements t_ℓ *knots* and the classical definition of the *B-spline of degree* d *with knot sequence* $t_{i:j}, j := i + d + 1$ is

$$B(x|t_{i:j}) := (t_j - t_i)\ \Delta(t_{i:j})(\max\{(\cdot - x), 0\})^d. \tag{3}$$

Here $\Delta(t_{i:j})$ acts on the function $h : t \to (\max\{(t-x), 0\})^d$ for a given $x \in \mathbb{R}$. Consequently, a B-spline is a non-negative piecewise polynomial function with support on the interval $[t_i..t_j)$. If μ is the multiplicity of the number t_ℓ in the sequence $t_{i:j}$, then $B(x|t_{i:j})$ is at least $d - \mu$ times continuously differentiable at t_ℓ.

[1] The survey [dB05] advertises the symbol Δ for divided differences over alternatives such as $[t_{i:j}]h$ or $h[t_{i:j}]$.

The Peano formula of the remainder term, when approximating a C^k-function by its kth order Taylor expansion, can be expressed in terms of a B-spline $B(t|t_{0:k})$ as (see e.g. [dB05])

$$\frac{1}{k!}\int_{\mathbb{R}} B(t|t_{0:k})g^{(k)}(t)dt = \Delta(t_{0:k})g. \tag{4}$$

An important step when deriving the constraint matrix for optimal SIAC spline coefficients is to re-interpret this formula as a convolution formula for B-splines with monomials.

Lemma 2.1 *For integers $k > 0$ and $\delta \geq 0$, and the alternating monomial $(-\cdot)^\delta$: $t \to (-t)^\delta$,*

$$\left(B(\cdot|t_{0:k}) * (-\cdot)^\delta\right)(x) = \binom{k+\delta}{k}^{-1} \Delta t_{0:k}(t-x)^{k+\delta}. \tag{5}$$

Proof For fixed x, we choose the function g in (4) to be $g := \binom{k+\delta}{\delta}^{-1}(\cdot - x)^{k+\delta}$. Then $g^{(k)}(t) = (k!)(t-x)^\delta$ and

$$\left(B(\cdot|t_{0:k}) * (-\cdot)^\delta\right)(x) =^{(1)} \int_{\mathbb{R}} B(t|t_{0:k})(-(x-t))^\delta dt = \frac{1}{k!}\int_{\mathbb{R}} B(t|t_{0:k})g^{(k)}(t)dt$$
$$=^{(4)} \Delta(t_{0:k})g = \binom{k+\delta}{k}^{-1} \Delta t_{0:k}(t-x)^{k+\delta}.$$

|||

We note that the divided difference in (5) applies to the variable t. Therefore $\Delta t_{0:k}(t-x)^{k+\delta}$ does not vary with t.

3 Optimal convolution coefficients

A spline SIAC convolution kernel $K : \mathbb{R} \to \mathbb{R}$ is a piecewise polynomial of degree d. The function K is considered optimal if

$$(K * (\cdot)^\delta)(x) = x^\delta, \qquad \delta = 0, \ldots, 2d, \tag{6}$$

i.e. if convolution of K with monomials reproduces the monomials up to degree $2d$. Specifically, optimal 2-sided SIAC spline filters take the form

$$K(x) := \sum_{\gamma=-d}^{d} c_\gamma B(x|t_{\gamma:\gamma+d+1}),$$

as a spline of degree d with leftmost knot t_{-d}. To satisfy the polynomial equations (6), we want to determine the coefficients $c_{-d:d}$ so that

$$\Big(\sum_{\gamma=-d}^{d} c_\gamma B(\cdot|t_{\gamma:\gamma+d+1}) * (-\cdot)^\delta\Big)(x) = (-x)^\delta, \qquad \delta = 0, \dots, 2d. \qquad (6')$$

Theorem 3.1 *The vector of optimal SIAC convolution coefficients* $\mathbf{c} := [c_{-d}, \dots, c_d]^{\mathtt{t}} \in \mathbb{R}^{2d+1}$ *is*

$$\mathbf{c} := M_0^{-1}\mathbf{e}_1, \qquad \textit{where} \qquad (7)$$

$$M_0 := \big[\Delta t_{\gamma:\gamma+d+1} t^{d+1+\delta}\big]_{\delta=0:2d,\gamma=-d:d}, \qquad \mathbf{e}_i(k) := \begin{cases} 1 & \textit{if } k = i \\ 0 & \textit{else }. \end{cases}$$

The matrix M_0 is of size $(2d+1) \times (2d+1)$ and the vector $\mathbf{e}_1$ picks out the first column of the inverse of M_0. The entries of M_0 depend on $t_{\gamma:\gamma+d+1}$, but not on t (and clearly not on x). The entry $M_0(r, \ell) \in \mathbb{R}$ in row $r \in 1 : 2d + 1$ and column $\ell \in 1 : 2d + 1$ is related to δ and γ by $\delta = r - 1$ and $\gamma = \ell - d - 1$.

Proof (of Theorem 3.1). By (5) of Lemma 2.1, the equation in (6') for the monomial of degree δ in $-x$ is equivalent to

$$\binom{d+1+\delta}{\delta}(-1)^\delta x^\delta = \big[\Delta t_{\gamma:\gamma+d+1}(t-x)^{d+1+\delta}\big]\big]_{\gamma=-d:d}\,\mathbf{c}. \qquad (6'')$$

In particular (6") has to hold for $x = 0$. Setting $x = 0$ in (6") and observing that, by convention, $\binom{d+1+\delta}{\delta} = 1$ for $\delta = 0$, we obtain the following system of $2d + 1 \times 2d + 1$ equations

$$\mathbf{e}_1 = \big[\Delta t_{\gamma:\gamma+d+1} t^{d+1+\delta}\big]_{\delta=0:2d,\gamma=-d:d}\,\mathbf{c} = M_0\mathbf{c}. \qquad (7')$$

Assume $[f_\delta] \in \mathbb{R}^{2d+1}$ is a left nullvector of M_0 and consider $f(t) := t^{d+1}\sum_{\delta=0}^{2d} f_\delta t^\delta$. The assuption implies that $\Delta t_{\gamma:\gamma+d+1} f = 0$ for $\gamma = -d : d$, which we may view as $d + 1$st level of a divided difference table. Completing the table up to degree $3d + 1$ fills it with zeros. Since $\Delta t_{\gamma:\gamma+d+1} t^{d+1+\delta} = \kappa_\delta\, \xi_\gamma^\delta$ for some $\xi_\gamma \in (t_\gamma..t_{\gamma+d+1}]$ this shows that f is of degree at most d. This is only possible if $f_\delta = 0, \delta \in \{0, 1, \dots, 2d\}$, i.e. there is no non-zero left nullvector; hence M_0 is (left-)invertible and $\mathbf{c} := M_0^{-1}\mathbf{e}_1$ is well-defined.

To show that $\mathbf{c}$ solves the *polynomial system* (6') for all x and not just $x = 0$, we define the $2d+1$ linearly independent functionals F_k, $k = 0, \dots, 2d$ as follows.

The functional F_k differentiates its argument k-times with respect to x and then evaluates the result at $x = 0$. Applying F_k to both sides of (6") yields a new system

$$M_k\mathbf{c} = \binom{d+1-k+\delta}{d+1} e_{k+1}, \qquad M_k(j,:) := \begin{cases} M_0(j-k,:), & \text{if } j > k, \\ 0, & \text{else,} \end{cases} \tag{6^k}$$

where $M_k(j,:)$ denotes the jth row of the matrix M_k. Since $M_k\mathbf{c} = M_k M_0^{-1}\mathbf{e}_1 = \mathbf{e}_{k+1}$ and $\binom{d+1-k+\delta}{d+1} = 1$ for $\delta = k$, we see that the choice $\mathbf{c} := M_0^{-1}\mathbf{e}_1$ satisfies all $2d+1$ systems of equations (6^k). This implies that the system of polynomial equations ($6'$) is satisfied by $\mathbf{c}$. $|||$

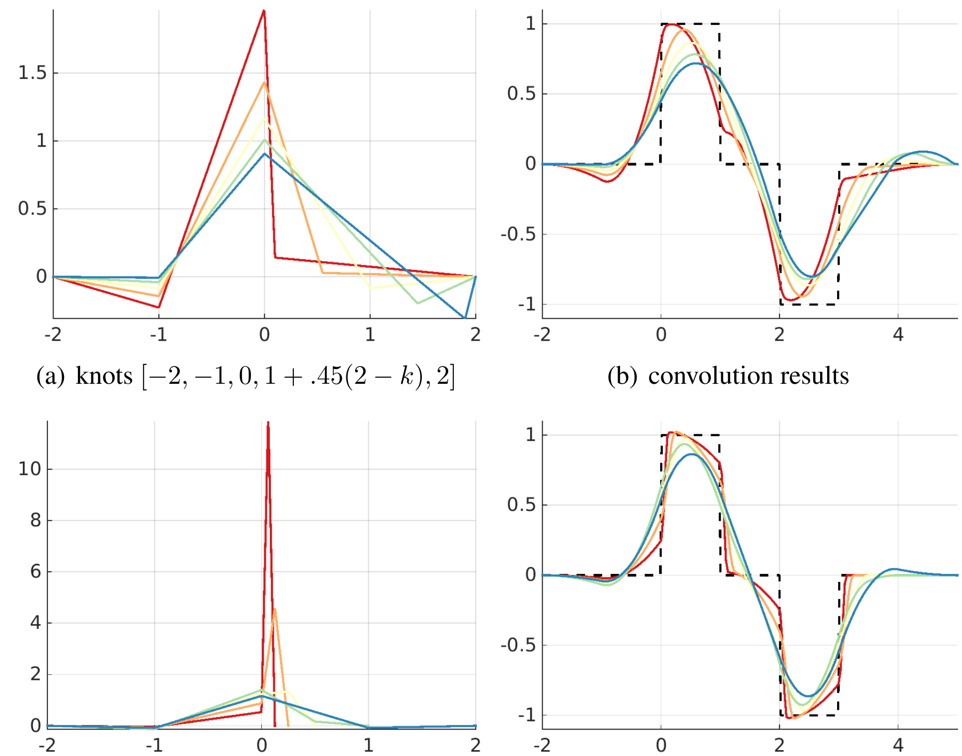
The entries of M_0 can be computed efficiently and stably via divided difference tables. We can modify the filter to read $K_j(x) := \sum_{\gamma=-d}^{j} c_\gamma B(x|t_{\gamma:\gamma+d+1})$. If we shorten the filter by choosing $j < d$ and retain the spline degree d, the number of columns of M_0 is reduced. If we remove accordingly the rows of M_0 above $d+1+j$, the proof of Theorem 3.1 is easily adapted to show that filter can reproduce monomials up to degree $j+d+1$. If we lengthen the filter by choosing $j > d$ and retain the spline degree d then we can reproduce monomials of degree exceeding $2d$ while keeping the smoothness of the convolved output the same. Distributing the knots asymmetrically yields asymmetric kernels. For example, moving the neighbor of the central knot closer as in Fig. 1a, increases the Gibbs undershoot on the left and reduces it on the right. Coalescing knots as in Fig. 1c allows, in the limit, to preserve jumps. When such effects are needed only locally, they can be blended with other kernels (see e.g. [vSRV11, RLKV14]).

4 Special knot sequences

If the knots are strictly increasing, we can expand the divided differences of monomials to make the expression for M_0 more explicit.

Corollary 4.1 (strictly increasing knots) *If, for $i = -d : 2d$, $t_i < t_{i+1}$ then*

$$M_0 = \left[\sum_{\ell=\gamma}^{\gamma+d+1} \frac{(-t_\ell)^{d+1+\delta}}{\prod_{j=\gamma,j\neq\ell}^{\gamma+d+1}(t_j - t_\ell)}\right]_{\delta=0:2d,\gamma=-d:d}. \tag{8}$$



(a) knots $[-2, -1, 0, 1 + .45(2 - k), 2]$

(b) convolution results

(c) knots $[-2, -1, 0, 2^{-k}, 2^{1-k}]$

(d) convolution results

Figure 1: Piecewise linear SIAC kernels (a,c) with asymmetrically-distributed knots for $k = 0, 1, 2, 3, 4$ convolved with a step signal (dashed) to yield (b,d).

(Multiplying the rows of M_0 by $(-1)^\delta$ reverses the sign of every second column of the inverse, but does not change the sign of the only relevant, first column.)

When the knot spacing is additionally uniform, i.e. $t_{i+1} - t_i = t_i - t_{i-1}$, then it is good to *symmetrize* it about 0. That is, we define $\gamma \in \tau := [-d - \sigma : d - \sigma]$, $\sigma := \frac{d+1}{2}$ so that the knot sequence is $[-d - \sigma : d + \sigma]$. For example, for $d = 1$, $\tau = [-2, -1, 0]$ and for $d = 2$, $\tau = [-3.5, -2.5, -1.5, -.5, 0.5]$. Then for $d = 2$, the knot sub-sequence defining the first B-spline is $[-3.5 : -0.5]$ and, symmetrically, the last knot sub-sequence is $[0.5 : 3.5]$.

Recently, Mirzargar [MR14] characterized the optimal symmetric SIAC kernel coefficients for uniform knots by the relations $\tilde{M}(x)\mathbf{c} = [x^\delta]_{\delta=0:2d}$, where

$$\tilde{M}(x) := \left[\sum_{\ell=0}^{\delta} (-1)^\ell \gamma^\ell \binom{\delta}{\ell} \left(B(\cdot|0:2d) * (\cdot)^{\delta-\ell}\right)(x)\right]_{\delta=0:2d, \gamma=-d:d}. \tag{9}$$

Specializing (8), we can remove the dependence on x.

Corollary 4.2 (uniform knots) *For uniform knots*

$$M_0 = \frac{1}{(d+1)!} \left[\sum_{\ell=0}^{d+1} (-1)^\ell \binom{d+1}{\ell} (\gamma+\ell)^{d+1+\delta}\right]_{\delta=0:2d, \gamma\in\tau}. \qquad (10)$$

The explicit form (10) makes it easy to prove the conjecture by Kirby and Ryan that the optimal SIAC coefficients in the uniform case are rational numbers: by Cramer's rule,

$$\mathbf{c}(i) = \frac{\det[M_0(:, 1:i-1), \mathbf{e}_1, M_0(:, i+1:2d+1)]}{\det M_0} \qquad (11)$$

and the determinants in the numerator and denominator only contain rational numbers.

For example, the optimal symmetric SIAC spline convolution coefficients for uniform knots and degree d are

$d=1:$ $[-1, 14, -1]/12,$

$d=2:$ $[37, -388, 2622, -388, 37]/1920,$

$d=3:$ $[-82, 933, -5514, 24446, -5514, 933, -82]/15120,$

$d=4:$ $[153617, -1983016, 12615836, -54427672, 180179750, \ldots]/92897280,$

$d=5:$ $[-4201, 61546, -437073, 2034000, -7077894, 18830604, \ldots]/7983360.$

where omitted entries in slots $d+2:2d+1$ indicated by "…" are defined by $c(d+1+i) = c(d+1-i)$. In [CLSS03], the middle entry for $d=2$ has the wrong sign.

5 Conclusion

For non-uniform knots, where pre-tabulation may not be practical, it is good to have explicit formulas for the entries of the optimal SIAC coefficient matrix M_0. These entries are computed stably and efficiently via divided difference tables. Tensoring the formulas yields multi-variate analogs. While the approximation space of the dG output and of the convolution operator need not agree and a tensor-product convolution kernel can be applied to piecewise polynomial output on tetrahedral meshes, when and how such multi-variate filters requires further study. The cost of convolution with *unstructured meshes*, already apparent in the uni-variate case, considerably increases the complexity of implementation and theoretical error analysis in the multi-variate setting. The generalized formulas should therefore be seen as *building blocks* for optimal non-uniform SIAC post-filtering.

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