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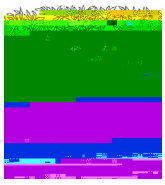

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On derivatives of smooth functions represented in multiwavelet bases ☆

Joel Anderson [a], Robert J. Harrison [a,*], Hideo Sekino [a], Bryan Sundahl [a], Gregory Beylkin [b]

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high-order derivatives of smooth functions represented in multiwavelet bases. During the development of various flavors of wavelet bases, multiwavelet bases were introduced perhaps as an afterthought. Initially, the whole thrust of wavelet constructions such as Daubechies wavelets [12] or spline wavelets (see e.g. [11]) was to ensure smoothness of a basis. Multiwavelets [1] appeared following a discrete wavelet-like construction

generalizing the Haar basis [17], multiwavelets kept the “unpleasant” feature that some basis functions are discontinuous. Counter-intuitively, as noted in [3], this feature may be considered “a blessing in disguise”. In particular, the fact that the scaling functions are supported on non-overlapping intervals allows high-order schemes on bounded intervals and, also, it is relatively easy to perform nonlinear operations. From an algorithmic point of view, it is also relatively easy to maintain a sparse representation of functions in higher dimensions when compared with required bookkeeping for overlapping bases. The observation that discontinuous basis functions allow high-order schemes is not unique to multiresolution bases as the same has been observed in, e.g., the discontinuous Galerkin methods. Consequently, since representations in multiwavelet bases have many useful properties and result in algorithms well suited for modern computer processors, they became a successful practical tool for high performance computing and are used in quantum chemistry [18,20,45,46] and nuclear physics [34,14,31,32], and serve as mathematical underpinnings of MADNESS [21].

Yet, the fact that basis functions are allowed to be discontinuous leads to a number of problems. As discussed in [3], the only scale-consistent derivative operator available to us is the first derivative. Operators for the second and higher derivatives do not exist due to the discontinuous nature of the basis and are applied as a power of the first derivative. Naively, if the function has high-order derivatives, such an approach appears reasonable. However, due to the approximate nature of representation in

make computations with functionals that incorporate derivatives more expensive compared to those that do not include derivatives. This is largely due to the need to compute much more accurately (i.e., oversample) in order to obtain accurate derivatives and function tails.

Another issue arising from the norm of the original derivative operator and the need to compute higher derivatives by its repeated application is that differential operators and their pseudo-inverse (i.e., convolution with the corresponding Green's function) do not numerically commute within the precision of computation — i.e., the order of operations matters and there is a lack of consistency between the numerical and formal calculus. This has emerged as a significant issue for scientists making first use of MADNESS, which typically requires reform /F3 e67.97-3.5(med1Tc ( ) Tm -.0125 Tc [(re)-12.7(q)11.2(u)-12.2(i)-12.8

other across all scales. Together, these relations enable the transformation between different scales of the multiresolution analysis. Note that at their mid-point the multiwavelets (4) are either discontinuous or have a discontinuous derivative.

The projection of a function $f(x)$ into the order-k scaling function basis at level n is

$$f^n(x) = \sum_{l=0}^{2^n-1} \sum_{j=0}^{k-1} s_{jl}^n \phi_{jl}^n(x). \tag{5}$$

where s are the scaling function coefficients. Assuming f is k-times differentiable, the approximation error is [1]

$$\left\| f - f^n \right\| \leq 2^{-nk} \frac{2}{4^k k!} \sup_{x \in [0,1]} \left| \frac{d^k}{dx^k} f(x) \right| \blacktriangle \tag{6}$$

Repeated application of the filters H^0, H^1, G^0 and G^1 (i.e., the fast wavelet

The construction preserves the 3-box stencil and scale-invariant operator, and hence can be used as a drop-in replacement in existing software (e.g., MADNESS [21], MRChem [25]).

We now explain our construction in a general setting that combines the projection and differentiation operators. Let us assume that we have two bases, the original basis $u_1(x), u_2(x), \ldots u_n(x)$ and an auxiliary basis $v_1(x), v_2(x), \ldots v_m(x)$, where $m \le n$ and the latter basis spans a subspace of the former (exactly or approximately within a given accuracy). Specifically, we are interested in the case where the basis functions $v_1, v_2, \ldots v_m$ all have derivatives of order p whereas not all of the functions $u_1(x), u_2(x), \ldots u_n(x)$ are p-differentiable. As we already pointed out, our main example is the basis where $u_1(x), u_2(x), \ldots u_n(x)$ are piece-wise polynomials.

We assume that the function f has the derivative of order p that we want to evaluate but is written in the original basis,

$$f(x) = \sum_{k=1}^{n} f_k u_k(x) + O(\epsilon). \tag{8}$$

where ϵ is the accuracy of computation. Note that if the coefficients f_k are known exactly then the error would be entirely in the wavelet spaces at the current and finer scales, but in practice the coefficients would only be known approximately.

Let us start by defining the $n \times m$ matrix $\mathbf{A}$ with entries

$$A_{il} = \int u_i(x) v_l(x)\, dx \tag{9}$$

and, if the original basis is not orthonormal, also the $n \times n$ Gram matrix $\mathbf{G}$ with entries

$$G_{ik} = \int u_i(x) u_k(x)\, dx, \quad i, k = 1, \ldots n.$$

Our first step is to project f on the subspace spanned by functions $v_1(x), v_2(x), \ldots v_m(x)$ reproducing in a least squares sense the projection onto the original basis. We seek the coefficients g_l so that

$$\sum_{k=1}^{n} f_k u_k(x) \approx \sum_{l=1}^{m} g_l v_l(x). \tag{10}$$

Denoting $\mathbf{f} = (f_1, f_2, \ldots f_n)$, $\mathbf{g} = (g_1, g_2, \ldots g_m)$ and projecting from the left with $u_i(x)$, we seek $\mathbf{g}$ such that

$$\mathbf{A}^T\mathbf{G}\mathbf{f} = \mathbf{A}^T\mathbf{A}\mathbf{g}.$$

Thus, we obtain coefficients of f in the auxiliary basis as

$$\mathbf{g} = \left(\mathbf{A}^T\mathbf{A}\right)^{-1}\mathbf{A}^T\mathbf{G}\mathbf{f}$$

and

$$\mathbf{D}^{(j)} = \mathbf{G}^{-1}\mathbf{B}^{(j)}\left(\mathbf{A}\mathbf{A}^{-1}\right)\mathbf{A}\mathbf{G}.$$

If the original basis $u_1, u_2, \ldots, u_n$ is orthonormal, then $\mathbf{G}$ is the identity matrix and we have

$$\mathbf{D}^{(j)} = \mathbf{B}^{(j)}\left(\mathbf{A}\mathbf{A}^{-1}\right)\mathbf{A}. \tag{11}$$

In our case the first basis consists of the multiwavelet scaling functions

where c (bandlimit) is a fixed parameter (see [5,6]). We seek (an approximate) basis for this space. While PSWFs can serve this purpose, it is more convenient in our case to use a fixed set of exponentials $\{e^{ic\xi_k x}\}_{k=1}^{M}$ as described in the sequel.

The use of band-limited functions on an interval for integration and interpolation relies on quadratures constructed in [44,5,33].[1] These Gaussian-type quadratures for bandlimited exponentials differ from the classical Gaussian quadratures for polynomials in that they are approximate. Indeed, with a finite number of nodes it is impossible to integrate exactly an infinite number of functions but, it turns out, that all functions $\mathcal{E}_c$ can be integrated within any finite user-selected accuracy ε. The generalized Gaussian quadratures for exponentials to integrate functions in $\mathcal{E}_c$ with accuracy ε are summarized as (see [5,33,6])

Lemma. *For $c > 0$ and any $\varepsilon > 0$, there exist a finite number of nodes $-1 \le \xi_1 < \xi_2 < \cdots < \xi_M \le 1$ and corresponding weights $w_k > 0$, such that for any $x \in [-1, 1]$,*

$$\left| \int_{-1}^{1} e^{ictx}\, dt - \sum_{k=1}^{M} w_k e^{ic\xi_k x} \right| \le \varepsilon. \tag{12}$$

where the number of nodes, $M = c + O(\log(1/\varepsilon))$, is (nearly) optimal. The nodes and weights maintain the natural symmetry, $\xi_k = -\xi_{M-k+1}$ and $w_k = w_{M-k+1}$.

We note that the construction of quadratures in [5,33] is more general than formulated here and yields quadratures for band-limited exponentials integrated with a weight function.

We now describe interpolation in $\mathcal{E}_c$. Given a finite accuracy ε, we seek to represent functions in $\mathcal{E}_c$ by a fixed set of exponentials $\{e^{ic\xi_k x}\}_{k=1}^{M}$, where M is as small as possible. It turns out (see [5]) that by finding quadrature nodes $\{\xi_k\}_{k=1}^{M}$ and weights $\{w_k\}_{k=1}^{M}$ for exponentials with bandlimit $2c$ and accuracy ε^2,

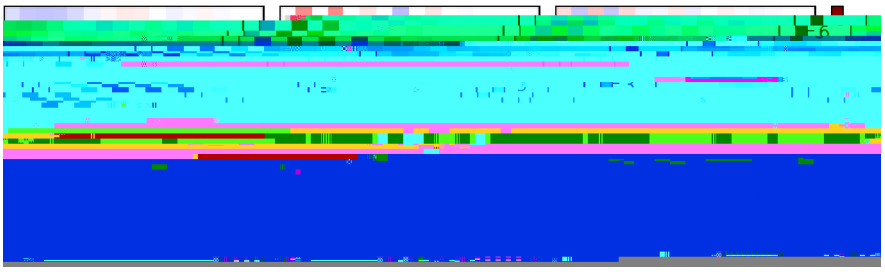

Fig. 1. Density plot of three blocks of the derivative matrix for $k = 16$ with a resulting accuracy of approximately 10^{-7}.

$[-1, -\frac{1}{3}]$, $[-\frac{1}{3}, \frac{1}{3}]$ and $[\frac{1}{3}, 1]$ with accuracy ϵ, where ϵ is the accuracy of representing exponentials in $\mathcal{E}_c$ via the basis functions.

Given a bandlimited (or approximately bandlimited) function in $\mathcal{E}_c$,

$$f(x) = \sum_{m=1}^{M} g_m e^{ic_m x}. \tag{13}$$

we denote the vector of its coefficients as $\mathbf{g} = \{g_m\}_{m=1}^{M}$. Using matrix $\mathbf{A}$, we obtain the coefficients of this function in the Legendre basis on the union

Table 1
For each of the

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