Approximations and Fast Algorithms

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ABSTRACT

The key element in the design of fast algorithms in numerical analysis and signal processing is the selection of an efficient approximation for the functions and operators involved.

In this talk we will consider approximations using wavelet and multiwavelet bases as well as a new type of approximation for bandlimited functions using exponentials obtained via Generalized Gaussian quadratures. Analytically, the latter approximation corresponds to using the basis of the Prolate Spheroidal Wave functions.

We will briefly comment on the future development of approximation techniques and the corresponding fast algorithms.

1. INTRODUCTION

Choosing a representation for functions and operators is the first and, perhaps, the most important step in any application. In signal processing such decisions often depend on the methodology of data collection. For example, most signals are treated as point values of functions. In numerical analysis different methods employ either point values or basis functions or both. An important consideration when making this choice is the quality of approximation within some class of functions depending on the number of allocated degrees of freedom (e.g., the number of points or coefficients used for approximation).

There is a great variety of bases one can choose from. We will concentrate on the question how the choice of basis affects algorithms for computing using such representations. Specifically, we review and compare smooth wavelet bases such as Daubechies' wavelets or spline wavelets, multiwavelets, and prolate spheroidal wave functions (PSWFs). These bases are quite different and the characteristic that distinguishes them and has most of the impact on the algorithms is the organization of the supports of the basis functions.

Most pairs of scaling functions and wavelets in Daubechies' bases have disjoint supports, but neighbors do overlap on a given scale, making it difficult to restrict the basis to an interval. The basis functions are localized in both time and frequency, and the improvement in resolution is achieved by the addition of basis functions with a smaller support. Spline bases (including spline wavelets) are very similar to Daubechies' bases in this regard but their orthogonalization produces infinite supports.

On the other hand, the scaling functions for multiwavelets and PSWFs on a collection of intervals are different in that they are organized in groups with the common support restricted to a particular interval. Since the intervals overlap with at most one point in the intersection, so do the supports of the corresponding groups of scaling functions. We emphasize that in considering multiwavelets we restrict ourselves to those developed by Alpert[1] following the construction of their discrete version.[2] From the point of view of this presentation, the overlapping multiwavelets developed later by several authors are *missing* the property that small groups of them have supports strictly limited to disjoint intervals, and we do not consider them here.

In other words, we consider two types of bases, those developed on the line and adapted (well or poorly) to the life on an interval, and those developed on the interval directly. We note that the bases on intervals are easily extended to the bases on the whole line by simply viewing the line as a collection of intervals.

The impact of basis selection on fast algorithms is both direct and subtle. The width of the bands in representing operators in wavelet bases is clearly basis dependent. On the other hand, the differences that follow from selecting bases with different organization of supports of basis functions is much less understood and we will discuss them here. In many applications it is advantageous to sacrifice smoothness of the basis functions in order to obtain disjoint supports and, as a result, certain high order numerical algorithms.

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2. BASES WITH SMOOTH FUNCTIONS.

The original goal of constructing wavelets was to find a smooth generalization of the Haar basis. It is, therefore, not surprising that some definitions of wavelets include the requirement that the basis functions are at least continuous. The smoothness is desireable to ensure sufficiently fast decay of the Fourier transform of the basis functions and, thus, their localization in the frequency domain. This goal has been achieved[19,15,10] and today there is a great variety of choices of such bases.[16,9]

Although it appears natural, the strategy of constructing smooth wavelets leads to a number of difficulties and limitations in the practical use of such bases. These difficulties appear in some signal processing applications but they are more pronounced in numerical analysis. Let us discuss the following three issues.

- The requirement of smoothness leads to the overlapping supports of the scaling functions on a given scale (consider splines as an example). As a consequence, it is necessary to adapt such bases to bases on an interval. Such constructions exist,[7,8] but necessarily involve boundary operators. The condition number of these operators grows rapidly with the order of the bases. As a result, such constructions in numerical analysis work satisfactorily for low order schemes but cause a loss of precision for high order schemes. In signal processing this problem appears where it is necessary to process finite data, for example, near the edge of an image. However, in most signal processing application the accuracy is low and it is acceptable to use a low order bases. In other words, in a low precision environment there are many acceptable ways to deal with the boundaries but the problem becomes much more difficult if high precision is required.

- In solving PDEs it is almost always necessary to perform the pointwise multiplication of functions. Therefore, it is very convenient to work with interpolating scaling functions. Let the subspace of a multiresolution analysis $\mathbf{V_0}$ be defined as a linear span of functions $\{\phi(x-n)\}_{n\in\mathbb{Z}}$, such that $\phi(n)=\delta_{n0}$. Then if $f\in\mathbf{V_0}$, we have

  $$f(x)=\sum_n f(n)\phi(x-n),$$

  or, in other words, coefficients of the expansion with respect to scaling functions are values of the function.

  However, the combination of smoothness, orthogonality and interpolating property leads to the non-compact support of the scaling functions. Interpolating bases are available, for example the Butterworth wavelets (named after the Butterworth filters, which happen to generate a multiresolution analysis). Since such bases do not have a compact support, it becomes even more difficult to adapt them to the life on an interval.

- Finally, the smoothness property limits the availability of scale consistent derivative operators. This is somewhat counterintuitive and we need to clarify this statement. The smoothness of the basis functions leads to the uniqueness of the representation of the derivative operator.[4] This simply follows from the absolute convergence of the integrals which define the coefficients of the representation. The coefficients of the representation on $\mathbf{V_0}$ are defined as

  $$r_l=\int_{-\infty}^{\infty}\phi(x-l)\,\frac{d}{dx}\,\phi(x)\,dx,$$

  and the integral is absolutely convergent for sufficiently smooth scaling functions.

  Once computed, such representation can be seen as a central difference operator and, because of the uniqueness, there is no analogue of forward and backward differences. For example, for Daubechies' wavelets with two vanishing moments, the coefficients $\{r_l\}_{l=-2}^{2}$ are $(-1/12, 2/3, 0, -2/3, 1/12)$. Naively, this does not appear as an inconvenience, but it turns out that in numerical analysis it is really useful to have forward and backward difference operators (for example, to easily impose the boundary conditions).

In combination these difficulties limit the use of bases with smooth functions in numerical analysis by essentially limiting the order of schemes for non-periodic problems. Although there are ways to overcome some of these difficulties,[5] overall it appears that smoothness of the bases functions comes with a high price tag in some applications.

3. POLYNOMIAL BASES ON AN INTERVAL.

Instead of a smooth generalization of the Haar basis, we can proceed in a different direction.[2,1] Such construction[1] was also suggested by Federbush[11] although not for numerical purposes.

The multiwavelet bases[1] retain the vanishing moment property but the basis function are not smooth at the point where intervals join and, in fact at least one of them always has a jump discontinuity similar to that of the Haar function.

It has been demonstrated that the discrete version of multiwavelets[2] and the polynomial version,[1] can both be successfully used for representing integral operators. A wide class of integrodifferential operators has effectively sparse representations in these bases, due to vanishing moments of the basis functions. An *effectively sparse* matrix representation is one that differs from a sparse matrix by a matrix with a small norm.

More recently, it has been demonstrated[3] that the multiwavelet bases are well suited for the high-order adaptive solvers of partial differential equations. Two of the issues raised in the consideration of bases with smooth functions, namely, the high-order accomodation of the boundary conditions and the availability of orthonormal bases with the interpolating property, are easily resolved using multiwavelets. On the third issue, the representation of differential operators in these bases, we note that there is a family of scale consistent derivative operators.[3] Such derivative operators may be viewed as (non-unique) weak representations. We view the non-uniqueness as an advantage rather than a deficiency since we have at our disposal a multiresolution generalization of finite difference schemes including that of the forward and backward differences. This is very convenient in a number of applications.

In the original construction,[1] the scaling functions $\phi_0, \ldots, \phi_{k-1}$ were chosen to be $\phi_j(x) = \sqrt{j+1/2}\, P_j(x)$, $j = 0, \ldots, k-1$, where P_j are the Legendre polynomials. These functions form an orthonormal basis for the space of polynomials of degree less than k on the interval [-1,1]. Alternatively, one can use interpolating polynomials as a basis for this space.

Given nodes $x_0, \ldots, x_{k-1}$, the Lagrange interpolating polynomials are defined as

$$l_j(x) = \prod_{\substack{i=0,\\ i \neq j}}^{k-1} \left(\frac{x - x_i}{x_j - x_i} \right), \qquad j = 0, \ldots, k-1, \tag{1}$$

and are characterized by $l_j(x_i) = \delta_{ij}$.

Given nodes $x_0, \ldots, x_{k-1}$ which are the roots of $P_k(x)$, and the associated Gauss-Legendre quadrature weights $w_0, \ldots, w_{k-1}$, the functions

$$R_j(x) = \frac{1}{\sqrt{w_j}} l_j(x), \qquad j = 0, \ldots, k-1, \tag{2}$$

have the following properties:

1. The functions $R_0, \ldots, R_{k-1}$ form an orthonormal basis on $[-1, 1]$ with respect to the inner product

$$\langle f, g \rangle = \int_{-1}^{1} f(x) g(x) dx. \tag{3}$$

2. For $j = 0, \ldots, k-1$, R_j is a linear combination of Legendre polynomials given by

$$R_j(x) = \sqrt{w_j} \sum_{i=0}^{k-1} \left(i + \frac{1}{2} \right) P_i(x_j) P_i(x). \tag{4}$$

3. Any polynomial f of degree less than k can be represented by the expansion

$$f(x) = \sum_{j=0}^{k-1} d_j R_j(x), \tag{5}$$

where the coefficients are given by $d_j = \sqrt{w_j} f(x_j)$, $j = 0, \ldots, k-1$.

Thus, up to rescaling, we have an interpolating basis of scaling functions.

The Legendre nodes $x_0, \ldots, x_{k-1}$ are not uniform and concentrate near the boundary. The condition numbers of boundary operators do not become large and the boundary conditions can be succesfully used for polynomials up to degree of about 30. For higher degrees, the concentration of the nodes near the ends of the interval start to create problems since the distances between the nodes are of order $O(1/k^2)$. Such spatial concentration of nodes also causes difficulties in time evolution schemes by restricting the size of time steps. Yet, the range of degrees is wide enough for practical purposes and significantly extends what can be done with mutiresolution bases PDE solvers.

Let us define $\mathbf{V}_n^k$ as a space of piecewise polynomial functions,

$$\begin{aligned} \mathbf{V}_n^k = \{ f : \quad & \text{the restriction of } f \text{ to the interval } (2^{-n}l,\ 2^{-n}(l+1)) \text{ is} \\ & \text{a polynomial of degree less than } k, \text{ for } l = 0, \ldots, 2^n - 1, \\ & \text{and } f \text{ vanishes elsewhere}\}. \end{aligned} \tag{6}$$

Let $\phi_0, \ldots, \phi_{k-1}$ be a basis of $\mathbf{V}_0^k$, then the space $\mathbf{V}_n^k$ is spanned by $2^n k$ functions which are obtained from $\phi_0, \ldots, \phi_{k-1}$ by dilation and translation,

$$\phi_{jl}^n(x) = 2^{n/2}\phi_j(2^n x - l), \qquad j = 0, \ldots, k-1, \quad l = 0, \ldots, 2^n - 1. \tag{7}$$

We define the multiwavelet subspace $\mathbf{W}_n^k$, $n = 0, 1, 2, \ldots$ as the orthogonal complement of $\mathbf{V}_n^k$ in $\mathbf{V}_{n+1}^k$,

$$\mathbf{V}_n^k \oplus \mathbf{W}_n^k = \mathbf{V}_{n+1}^k, \qquad \mathbf{W}_n^k \perp \mathbf{V}_n^k. \tag{8}$$

The multiwavelets are introduced as piecewise polynomial functions $\psi_0, \ldots, \psi_{k-1}$ which form an orthonormal basis for $\mathbf{W}_0^k$,

$$\int_0^1 \psi_i(x)\psi_j(x)dx = \delta_{ij}. \tag{9}$$

Since $\mathbf{W}_0^k \perp \mathbf{V}_0^k$, the first k moments of $\psi_0, \ldots, \psi_{k-1}$ vanish,

$$\int_0^1 \psi_j(x)x^i dx = 0, \qquad i, j = 0, 1, \ldots, k-1\,. \tag{10}$$

The space $\mathbf{W}_n^k$ is spanned by $2^n k$ functions obtained from $\psi_0, \ldots, \psi_{k-1}$ by dilation and translation,

$$\psi_{jl}^n(x) = 2^{n/2}\psi_j(2^n x - l), \qquad j = 0, \ldots, k-1, \quad l = 0, \ldots, 2^n - 1, \tag{11}$$

The condition of orthonormality of $\psi_0, \ldots, \psi_{k-1}$ yields

$$\int_0^1 \psi_{il}^n(x)\psi_{jm}^{n'}(x)dx = \delta_{ij}\delta_{lm}\delta_{nn'}. \tag{12}$$

These conditions leave a significant freedom in choosing the multiwavelets. Let us mention two natural choices. First is to select the basis so to maximize the number of vanishing moments for some of the basis functions.[1] Alternatively, one can organize the functions by the type of singularity, that is, to have one basis function with jump discontinuity, next with jump discontinuity in the first derivative, etc.

The relations between the subspaces may be expressed by the two-scale difference equations,

$$\phi_i(x) = \sqrt{2}\sum_{j=0}^{k-1}\left(h_{ij}^{(0)}\phi_j(2x) + h_{ij}^{(1)}\phi_j(2x-1)\right), \qquad i = 0, \ldots, k-1, \tag{13}$$

$$\psi_i(x) = \sqrt{2}\sum_{j=0}^{k-1}\left(g_{ij}^{(0)}\phi_j(2x) + g_{ij}^{(1)}\phi_j(2x-1)\right), \qquad i = 0, \ldots, k-1, \tag{14}$$

where the coefficients $h_{ij}^{(0)}, h_{ij}^{(1)}$ and $g_{ij}^{(0)}, g_{ij}^{(1)}$ depend on the choice of the order k and are readily computed once the bases for $\mathbf{V}_0^k$ and $\mathbf{W}_0^k$ have been chosen.[3]

The scale consistent derivative operator on $\mathbf{V}_0^k$ is constructed as a transition matrix R^n between the coefficients of the expansion of the function and that of its derivative. The scale consitency means that on $\mathbf{V}_n^k$ the transition matrix is simply rescaled by 2^n since the derivative operator is homogeneous of degree one. The transition matrix R^n has a block tridiagonal structure

$$R^n = \begin{pmatrix} r_0 & r_{-1} & & \\ r_1 & \ddots & \ddots & \\ & \ddots & \ddots & r_{-1} \\ & & r_1 & r_0 \end{pmatrix}, \tag{15}$$

each block r_l being a $k \times k$ matrix. The matrix blocks r_1 and r_{-1} describe interactions with the left and the right neighboring intervals, respectively, and have rank one as matrices. There are two free parameters associated with the two neighboring intervals, and these define the family of transition matrices. By choosing these parameters, the blocks r_1 or r_{-1} can be made zero, thus providing us with an analogue of forward and backward differences.[3] It is easy to impose a linear boundary condition since such condition amounts to supplying a value to one of the free parameters. The boundary operators have a reasonable condition number since we effectively are using the Gauss-Legendre nodes on the interval (to make it obvious, consider the interpolating scaling functions). The classical Runge example for interpolation then demonstrates the benefits of the Gauss-Legendre nodes versus the equally spaced nodes (which is equivalent to using the usual Multiresolution Analysis and smooth basis functions).

This multiwavelet approach has been used to build an adaptive multiresolution PDE solver for advection-diffusion equations[3] and currently work is under way to develop such solver in multiple dimensions.

4. OPTIMAL BASES ON AN INTERVAL

We now turn to the prolate spheroidal wave functions (PSWFs) introduced by Slepian et. al.[18,14]

The PSWFs are defined as the eigenfunctions of the operator $F_c : L^2[-1,1] \to L^2[-1,1]$,

$$F_c(\phi)(x) = \int_{-1}^{1} \mathrm{e}^{\mathrm{i}cxt}\, \phi(t) dt, \tag{16}$$

where c is a positive real constant (bandlimit). The PSWFs satisfy

$$\lambda_j \psi_j(x) = \int_{-1}^{1} \mathrm{e}^{\mathrm{i}cxt}\, \psi_j(t) dt, \tag{17}$$

where the eigenvalues λ_j, $j = 0, 1, \ldots$, are all non-zero and simple, and are arranged so that $|\lambda_j| > |\lambda_{j+1}|$, $j = 0, 1, 2, \ldots$. The eigenvalues λ_j are either real or pure imaginary depending on the parity of the eigenfunction ψ_j. These eigenfunctions are also eigenfunctions of the operator $Q_c = \frac{c}{2\pi} F_c^* F_c$ and satisfy

$$\mu_j \psi_j(x) \;=\; \frac{1}{\pi} \int_{-1}^{1} \frac{\sin c(x-t)}{(x-t)}\, \psi_j(t) dt, \tag{18}$$

with eigenvalues

$$\mu_j = \frac{c}{2\pi} |\lambda_j|^2, \quad j = 0, 1, \ldots. \tag{19}$$

For large c the first approximately $2c/\pi$ eigenvalues μ_j are close to 1. They are followed by $O(\log c)$ eigenvalues which decay exponentially fast from 1 to almost zero. The rest of the eigenvalues are very close to zero.

There also exists a strictly increasing sequence of real numbers $\eta_0 < \eta_1 \ldots$, such that ψ_j in (17) are eigenfunctions of the differential operator,[18]

$$L\psi_j \equiv \left(-(1-x^2) \frac{d^2}{dx^2} \;+\; 2x \frac{d}{dx} \;+\; c^2 x^2 \right) \psi_j(x) \;=\; \eta_j \psi_j(x)\,. \tag{20}$$

The eigenfunctions of L have been known as the angular prolate spheroidal functions before the connection with (17) was discovered.[18] We note that if $c \to 0$, then it follows from (20) that ψ_j become the Legendre polynomials in this limit.

For any $n \geq 0$, the first n functions ψ_j, $j = 0, \ldots, n-1$, form a Chebyshev system.[12,13] In particular, the number of zeros of ψ_j in $[-1, 1]$ is equal to j.

Although the functions ψ_j are defined on the interval, they are easily extended to the whole line using the right hand side of (18) as the definition of the extension. The functions ψ_j are orthogonal on both the interval $[-1, 1]$ and the real line $(-\infty, \infty)$, and we set

$$\int_{-1}^{1} \psi_j(x)\, \psi_l(x)\, dx = \delta_{jl}\,, \tag{21}$$

and

$$\int_{-\infty}^{\infty} \psi_j(x)\, \psi_l(x)\, dx = \frac{1}{\mu_j}\delta_{jl}\,. \tag{22}$$

We note that in the original papers[18,14,17] the functions are chosen to be orthonormal on $(-\infty, \infty)$.

From definition (17) it follows that

$$\mathrm{e}^{\mathrm{i}cxt} = \sum_{j=0}^{\infty} \lambda_j\, \psi_j(x)\psi_j(t)\,. \tag{23}$$

If we keep $\approx 2c/\pi + K \log c$ terms, where $K = K(\epsilon)$ is a constant, we obtain (for any $\epsilon > 0$) an approximation to $\mathrm{e}^{\mathrm{i}cxt}$. This is the most economical expansion of this type for the exponential.

The PSWFs have been used in signal processing for some time, especially the first function, $\psi_0(x)$, since it provides the optimal window for a given bandwidth in terms of concentration in the time-frequency domain. Yet, their use has not been wide. In the next section we describe several new developments that will provide a path for a wider use of these functions in signal processing and numerical analysis.

5. GENERALIZED GAUSSIAN QUADRATURES FOR EXPONENTIALS

The generalized Gaussian quadratures for exponentials has been developed recently.[20,6] Within the first approach,[20] the authors construct the generalized Gaussian quadratures for the prolate spheroidal wave functions using the fact that the first n of these functions form a Chebyshev system,[12,13] for any n. For a given accuracy ϵ and a choice of n, these quadratures are also quadratures for exponentials due to (23). Alternatively, a new type of the generalized Gaussian quadratures for exponentials has been obtained directly[6] and these quadratures are parameterized by eigenvalues of the Toeplitz matrix constructed from the trigonometric moments of a positive measure. For a given accuracy ϵ, selecting an eigenvalue close to ϵ yields an approximate quadrature for that accuracy. These quadratures can be used to approximate and integrate other essentially bandlimited functions, for example, Bessel functions and prolate spheroidal wave functions.

Let us define the bandlimited functions with the bandlimit c as a class of functions that can be represented via a linear combination of exponentials $\exp(\mathrm{i}b\,x)$ with e.g., l^1-bounded coefficients, where b is *any* real number, $|b| \leq c$.

It turns out, that for any accuracy $\epsilon > 0$ and any bandlimit $c > 0$, there is a set of M functions, $\{\exp(\mathrm{i}ct_k\, x)\}_{k=1}^{M}$, where the nodes $t_k = t_k(\epsilon, c)$, $|t_k| < 1$, and the coefficients $\alpha_k = \alpha_k(b)$, are such that

$$|\exp(\mathrm{i}b \cdot x) - \sum_{k=1}^{M} \alpha_k(b) \exp(\mathrm{i}ct_k\, x)| \leq \epsilon\,. \tag{24}$$

The set of functions $\{\exp(\mathrm{i}ct_k\, x)\}_{k=1}^{M}$ can be viewed as an approximate basis.

In order to find the nodes t_k in (24), we solve the following problem[6] described here in a slightly more general setting that is need to obtain (24). Let us consider integrals of the form

$$u(x) = \int_{-1}^{1} \exp(2c\,t\,x)\, d\mu(t), \tag{25}$$

where $d\mu(t)$ is a measure, typically $d\mu(t) = w(t)dt$, where w is a weight function, namely, w is a real, non-negative, integrable function with $\int_{-1}^{1} w(\tau)d\tau > 0$. To obtain (24) the weight is set $w = 1$.

For a given bandlimit $2c > 0$ and accuracy $\epsilon^2 > 0$, we approximate $u(x)$ on the interval $[-1, 1]$ using the sum

$$\tilde{u}(x) = \sum_{k=1}^{M} w_k \exp(2c\, t_k\, x), \tag{26}$$

where $w_k > 0$ and $M = M(c, \epsilon^2)$, so that

$$|u(x) - \tilde{u}(x)| \le \epsilon^2 \quad \text{for} \quad x \in [-1, 1]. \tag{27}$$

The number of terms, M, is optimal. Solving this problem involves finding the eigenvalues and eigenvectors of the Toeplitz matrix constructed using the values of $u(x)$ discretized at the equally spaced nodes and interpreted as the trigonometric moments of a positive measure.[6]

Once the nodes are computed, the set of functions $\{\exp(\mathrm{i}ct_k\, x)\}_{k=1}^{M}$ can serve as an approximate basis on the interval $[-1, 1]$ in (24). Such bases can be organized into a hierarhical structure similar to multiwavelets. We will report these results elsewhere.

The representation in (24) retains the property of disjoint support similar to that of multiwavelet bases. On the other hand, it requires significantly fewer terms than the representation with orthogonal polynomials. Also, one can think of the bandlimit c as an analogue of the degree in the case of polynomials and, unlike in that case, there is no constraint on the bandwidth c. This is because the distance between the nodes is $O(1/c)$ and, thus, the quadrature nodes do not significantly concentrate near the ends of the interval as, for example, the Legendre nodes. These properties of the representations using exponentials lead to a number of new algorithms that are being developed and will be presented elsewhere.

6. CONCLUSIONS

As we can see, the development of bases came a full circle, coming back to the prolate spheroidal wave functions first introduced in early sixties. These functions are constructed specifically on the interval and are more efficient there than the polynomials. Yet, their use has been limited for a number of reasons. With the advent of generalized Gaussian quadratures for the prolate spheroidal wave functions and the exponentials, the situation will changes and we anticipate a wider use of them in a number of applications.

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