

**A Multiresolution Approach to  
Fast Summation  
and  
Regularization of Singular Operators**

by

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Thesis directed by Professor Gregory Beylkin

A class of fast algorithms is introduced for the evaluation of discrete sums that utilizes projections on a multiresolution analysis. The discrete sums under consideration arise, for example, in the study of physical systems by means of particle simulations requiring long-range potentials. These include gravitational and electrostatic models, plasma physics, atmospheric physics, and vortex methods in fluid dynamics. These numerical models of particle interactions require the application of dense matrices which, done directly, requires  $O(N^2)$  arithmetic operations. The algorithms we develop accomplish this task to within accuracy  $\epsilon$  in  $O(N)$  arithmetic operations.

There are two types of algorithms used today for the fast computation of discrete sums, namely, the Method of Local Corrections and the Fast Multipole Method. Our approach is related to both, but has its own unique features. We describe implementations in one and two dimensions, and present theoretical foundations for algorithms in higher dimensions.

In our approach to discrete summation problems, we construct explicit representations of singular operators on subspaces of the multiresolution analysis. These representations provide a definition for the regularization of such operators, as well as a practical algorithm for their computation. We present a new multiresolution approach to the regularization of singular operators, and show that our method coincides with the classical method, where the classical method is applicable.

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# chapter 1

## Introduction

### 1.1 Introductory Remarks

The study of physical systems by means of particle simulations is an important computational tool in many fields. Examples include plasma physics, atmospheric physics, N-body gravitational problems, and vortex methods in fluid dynamics. In most of these particle models the evaluation of discrete sums describing the pairwise interactions between particles occupies a central role, and is often the most expensive part of the computation. Discrete sums may also be encountered in the evaluation of integral equations obtained in the solution of boundary value problems. In any event, numerical models require the application of dense matrices which, done directly, requires an amount of work proportional to  $N^2$  for an  $N$  particle system (or  $N$  point discretization). To overcome this computational hurdle there is a need for fast  $O(N)$  algorithms.

In this thesis, we introduce a class of fast algorithms for the computation of discrete sums using projections on a multiresolution analysis. (A brief

As a special case of (1.1) we consider the sums

$$g(x_m) = \sum_{\substack{n=1 \\ n \neq m}}^N K(x_m - x_n) f(x_n), \quad 1 \leq m \leq N \quad (1.2)$$

here the  $N$  sampling locations coincide with the positions of the  $N$  particles. Indeed, there is no loss of generality in taking (1.2) as our model problem, and this we do from now on. The particle locations  $\{x_n\}_{n=1}^N$  are points in  $\mathbf{R}^d$ , here



In our approach to discrete summation problems, we construct explicit representations

for some positive  $\delta$ . It follows from (1.7) that  $|K_{HF}(x, y)|$  decays rapidly as  $|x - y|$  increases. Therefore, this singular part of the kernel influences only the short range, or local interactions, and is represented by a banded matrix which can be applied to a vector in  $O(N)$  operations.

### 1.3 A B

Implicit in the FMM is the simple splitting  $K = K_{LF} + K_{HF}$ , here

$$K_{LF} = \begin{cases} 0, & |x - y| \leq \delta \\ K(x - y), & |x - y| > \delta \end{cases} \quad \text{and} \quad K_{HF} = \begin{cases} K(x - y), & |x - y| \leq \delta \\ 0, & |x - y| > \delta \end{cases}$$

The low frequency part is applied by a clever use of multipole expansions in a divide and conquer strategy, taking advantage of the smoothness of the kernel on regions removed from the origin to truncate the expansions after a few terms. The high frequency part is applied directly. Despite its apparent simplicity, the algorithm is not so straightforward to implement. The explicit form of the multipole expansions and translation operators, which are responsible for shifting the expansions from one box center to another, must be worked out anew for each new kernel. However, when properly implemented, the FMM provides a very efficient  $O(N)$  algorithm.

The Method of Local Corrections was introduced in [1] as a vortex method for solving problems in fluid mechanics, though the main ideas are certainly relevant in a more general context. This method is designed to approximate the velocity field due to a distribution of “vortex blobs” in a fluid, and to evaluate this field at the center of each blob. A vortex blob is a radially symmetric function, usually with compact support, that approximates a point vortex. In [1] it is observed that “...the difference between the velocity field due to a point vortex and a vortex blob located at the same point in space becomes very small as one moves away from the center of the vortices.” (This statement should be compared to the error estimate (1.8).) The approximate velocity is first obtained on an equispaced grid via a fast Poisson solver (FFT), and then interpolated to the centers of the vortices. The approximation is then corrected locally, for all vortices that lie in close proximity to other vortices. The interpolation is accomplished by the use of a complex-valued interpolating polynomial, made possible by the fact that the  $x$ - and  $y$ - components of velocity are the real and imaginary parts of a harmonic function. This is a special feature of vortex methods, and is not likely to generalize to other applications. The correction step in this method is essentially equivalent to (1.7), and the splitting of the kernel is achieved by means analogous to that described in Section 1.2. However, in approximating the velocity field, a smoothed version of the original operator is not constructed, and a finite difference method is employed instead.

In [11], a class of algorithms for particle simulations involving Poisson’s equation is developed. These algorithms are named PPPM by the authors, which stands for “particle-particle, particle-mesh.” The name refers to the by now familiar splitting of the summation into low and high frequency contributions. The low frequency part is evaluated on an equispaced grid, or mesh. The values assigned to the mesh points are obtained from the charges on the particles by use of a fast multipole



# Chapter 2

## Multiresolution Analysis

### 2.1 Definition and Basic Properties

We first make some preliminary comments. Throughout this thesis, we use the notation  $\hat{f}$  to refer to the Fourier transform of a function  $f$ ,

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} e^{ix \cdot \xi} f(x) dx, \quad f(x) = \frac{1}{(2\pi)^d} \int_{-\infty}^{\infty} e^{-ix \cdot \xi} \hat{f}(\xi) d\xi.$$

for a function  $f \in L^2(\mathbf{R}^d)$ . We use  $(\cdot, \cdot)$  to refer to the usual inner product on  $L^2(\mathbf{R}^d)$ ,

$$(f, g) = \int_{-\infty}^{\infty} f(x) \overline{g(x)} dx.$$

A superscript and a subscript on a function will denote, respectively, a dilation and a translation,

$$f_k^j(x) = 2^{-dj/2} f(2^{-j}x - k),$$

here  $j \in \mathbf{Z}$  and  $k \in \mathbf{Z}^d$ . This will sometime

In what follows, we make repeated use of Poisson's summation formula,

$$\sum_{k=-\infty}^{\infty} f(k)e^{ik\xi} = \sum_{l=-\infty}^{\infty} \hat{f}(\xi + 2l\pi). \quad (2.1)$$

There exist many proofs of this well-known result (see e.g. [18] or [22]).

The following definition is by no means standard, and is borrowed from [20, p.21].

**Definition 2.1.1** *A multiresolution approximation of  $L^2(\mathbb{R})$*

The







**Proof:** The moments of  $\Phi$  are given in terms of the Fourier transform by the formula

$$\int_{-\infty}^{\infty} x^m \Phi(x) dx = (-i)^m \hat{\Phi}^{(m)}(0)$$

here  $\hat{\Phi}^{(m)}$  denotes the  $m$ th derivative of  $\hat{\Phi}$ . From (2.15) it follows that  $\hat{\Phi}(0) = 1$  since  $\hat{\phi}(0) = 1$ . By differentiating both sides of (2.16) we obtain

$$2^m \hat{\Phi}^{(m)}(2\xi) = \sum_{n=0}^m \binom{m}{n} \hat{\Phi}^{(m-n)}(\xi) M_0^{(n)}(\xi).$$

When  $\xi = 0$ , we have

$$\hat{\Phi}^{(m)}(0) = \frac{1}{2^m - 1} \sum_{n=1}^m \binom{m}{n} \hat{\Phi}^{(m-n)}(0) M_0^{(n)}(0). \quad (2.20)$$

Differentiating (2.18), we obtain

$$M_0^{(n)}($$

In order to compute the moments of the scaling function, it is not necessary to evaluate the defining integral,

$$\mu_m = \int_{-\infty}^{\infty} x^m \phi(x) dx.$$

Instead, we have the following recursive formula

$$\begin{aligned} \mu_0 &= 1, \\ \mu_m &= \frac{1}{2^m - 1} \sum_{n=1}^m \binom{m}{n} \nu_n \mu_{m-n}, \quad m \geq 1 \end{aligned} \quad (2.22)$$

here

$$\nu_n = \frac{1}{\sqrt{2}} \sum_l l^n h_l.$$

The numbers  $\{\nu_n\}$  are the (normalized) moments of the sequence  $\{h_l\}$ , and are easily computed when  $\{h_l\}$  is of finite length.

The formula (2.22) is well-known and is derived as follows. Using the two-scale difference equation (2.8), we have

$$\begin{aligned} \mu_m &= \int x^m \phi(x) dx \\ &= \sqrt{2} \sum_l h_l \int x^m \phi(2x - l) dx \\ &= \frac{1}{\sqrt{2}} \sum_l h_l \int \left(\frac{x+l}{2}\right)^m \phi(x) dx \\ &= \frac{1}{2^m} \sum_{n=0}^m \binom{m}{n} \frac{1}{\sqrt{2}} \sum_l l^n h_l \int x^{m-n} \phi(x) dx \\ &= \frac{1}{2^m} \sum_{n=0}^m \binom{m}{n} \nu_n \mu_{m-n}, \end{aligned}$$

from which (2.22) easily follows. Since  $\mathbf{y} \in \mathbb{P}^d \subset \mathbb{P}^d$

Thus, the two-scale difference equation for  $\Phi$  may be expressed in terms of the variable  $x$  as

$$\Phi(x) = \frac{1}{2} \sum_m a_m \Phi(2x - m). \quad (2.25)$$

Setting  $x = n$ ,  $n \in \mathbf{Z}$  we have

$$\Phi(n) = \frac{1}{2} \sum_m a_m \Phi(2n - m).$$

The interpolating property (2.14) implies that  $a_{2n} = 2\delta_{n,0}$ , here  $\delta$  denotes the Kronecker delta. Using (2.24) it is easy to show that  $a_{-m} = a_m$ , and we use these observations to write

$$\Phi(x) = \Phi(2x) + \frac{1}{2} \sum_{m \geq 1} a_{2m-1} [\Phi(2x - 2m + 1) + \Phi(2x - 1 + 2m)]. \quad (2.26)$$

If  $\Phi$  is compactly supported, as it must be if  $\phi$  has compact support, then we understand that only finitely many of the coefficients in (2.26) are non-zero.

### 2.1.4 Examples

Perhaps the simplest example of an MRA is one whose elements are piecewise constant on dyadic intervals. The scaling function for this MRA is the characteristic function of the interval  $[0, 1)$ ,

$$\phi(x) = \begin{cases} 1, & 0 \leq x < 1 \\ 0, & \text{otherwise.} \end{cases} \quad (2.27)$$

For historical reasons this is known as the Haar system. The Fourier transform is

$$\begin{aligned} \hat{\phi}(\xi) &= \int_0^1 e^{ix\xi} dx = \frac{e^{i\xi} - 1}{i\xi} \\ &= \left( \frac{e^{i\xi/2} - 1}{i\xi/2} \right) \left( \frac{e^{i\xi/2} + 1}{2} \right) \\ &= \hat{\phi}(\xi/2) m_0(\xi/2). \end{aligned}$$

From this expression, we can read off the trigonometric polynomial  $m_0$ , i.e.

$$m_0(\xi) = \left( \frac{1 + e^{i\xi}}{2} \right) = \frac{1}{\sqrt{2}} \sum_l h_l e^{il\xi},$$

which implies that  $h_0 = h_1 = 1/\sqrt{2}$ , and  $h_l = 0$  otherwise. Furthermore, from the explicit form of  $m_0(\xi)$ , we see that this function has a single zero at  $\xi = \pi$ .

The two-scale difference equation satisfied by (2.27) is

$$\phi(x) = \phi(2x) + \phi(2x - 1).$$

The autocorrelation of (2.27) is

$$\Phi(x) = \begin{cases} 1 + x, & -1 \leq x < 0 \\ 1 - x, & 0 \leq x < 1 \\ 0, & \text{otherwise.} \end{cases}$$

It is easily verified that

$$\int_{-\infty}^{\infty} \Phi(x) dx = 1, \quad \int_{-\infty}^{\infty} x\Phi(x) dx = 0.$$

Example(1) is the lowest order member of both families of scaling functions mentioned in this thesis, namely the central B-splines and the orthonormal scaling functions with compact support constructed by Daubechies (see [7] or [8]). Spline spaces will be described in more detail in Section 2.4. Daubechies scaling functions satisfy the two-scale difference equation

$$\phi(x) = \sqrt{2} \sum_{l=0}^{2M-1} h_l \phi(2x - l), \quad \text{here } \sum_{l=0}^{2M-1} h_l^2 = 1.$$

This scaling function provides an orthonormal basis for the subspaces of an MRA with  $M$  vanishing moments, for  $M = 1, 2, \dots$ , here  $M$  is the multiplicity of the zero at  $\xi = \pi$  in (2.12). The support of  $\phi$  is the interval

These scaling functions possess good approximation properties, but are difficult to evaluate point

for  $0 \leq m \leq M - 1$ .

Due to our assumption of compact support or exponential decay at infinity, the numbers  $\mu_m$  are well-defined for every integer  $m \geq 0$ . Before giving the proof of the proposition, we state and prove a series of lemmas.

**Lemma 2.2.1** *If  $\phi(x)$  is compactly supported or satisfies (2.31), then for each non-negative integer  $m$  there exists a constant  $C_m$  such that*

$$\sum_{k=-\infty}^{\infty} |x - k|^m |\phi(x - k)| \leq C_m \quad (2.33)$$

for every real  $x$ , and the sum converges uniformly.

**Proof:** First assume that  $\phi(x)$  is compactly supported. No

$$\sum_{k=-\infty}^{\infty} |x - k|^m |\phi(x - k)| = \lim_{N \rightarrow \infty} \sum_{k=-N}^N |x - k|^m |\phi(x - k)|,$$

provided that this limit exists. If the limit exists, then the limit function must be 1-periodic, so it is sufficient to consider  $0 \leq x < 1$ . Let  $[a, b]$  be the smallest closed interval that contains the support of  $\phi(x)$ . Then  $\phi(x - k) = 0$  if  $x - k > b$  or  $x - k < a$ , so it follows that

$$\lim_{N \rightarrow \infty} \sum_{k=-N}^N |x - k|^m |\phi(x - k)| = \sum_{k=k_0}^{k_1} |x - k|^m |\phi(x - k)|,$$

here  $k_0 = -\lfloor b \rfloor$ ,  $k_1 = -\lfloor a \rfloor$ , and  $\lfloor \cdot \rfloor$  denotes the greatest integer less than or equal to  $(\cdot)$ . Thus the sequence of partial sums converges for each  $x$ , and as the sum involves only a finite number of terms it converges uniformly. For  $0 \leq x < 1$ , we have  $|k| \leq |x - k| \leq |k| + 1$ , so that

$$\sum_{k=k_0}^{k_1} |x - k|^m |\phi(x - k)| \leq \|\phi\|_{\infty} \sum_{k=k_0}^{k_1} (1 + |k|)^m, \quad (2.34)$$

here  $\|\phi\|_{\infty} = \sup |\phi(x)|, a \leq x \leq b$ . It follows that the sum is uniformly bounded by the constant on the right-hand side of (2.34).

Next assume that  $\phi(x)$  has exponential decay at infinity, i.e.  $|\phi(x)| \leq Ae^{-\alpha|x|}$ , for some positive constants  $A$  and  $\alpha$ . No

$$\sum_{k=-\infty}^{\infty} |x - k|^m |\phi(x - k)| = \lim_{N \rightarrow \infty} \sum_{k=-N}^N |x - k|^m |\phi(x - k)|,$$

provided that this limit exists, and as before it is sufficient to consider  $0 \leq x < 1$ . Then  $|k| \leq |x - k| \leq |k| + 1$  implies that

$$|x - k|^m |\phi(x - k)| \leq A|x - k|^m e^{-|x-k|} \leq A(1 + |k|)^m e^{-|k|}.$$

Thus,

$$\sum_{k=-N}^N |x - k|^m |\phi(x - k)| \leq A \sum_{k=-N}^N (1 + |k|)^m e^{-|k|}, \quad (2.35)$$

and as  $N \rightarrow \infty$  the sequence of partial sums on the right converges for any non-negative integer  $m$ . It follows that the sequence of partial sums on the left-hand side of (2.35) converges uniformly for each  $x$ , and the limit function is uniformly bounded by the constant  $A \sum_{-\infty}^{\infty} (1 + |k|)^m e^{-|k|}$ .  $\square$

**Lemma 2.2.2** *If  $\phi(x)$  is compactly supported or satisfies (2.31), then  $x^m \phi(x)$  is in  $L^1(\mathbf{R})$  for each non-negative integer  $m$ , and we have the estimate*

$$\int_{-\infty}^{\infty} |x|^m |\phi(x)| dx \leq C_m, \quad (2.36)$$

where the constants in (2.33) and (2.36) are identical  $A$



here ^

No assume that  $\hat{\phi}^{(n)}(2l\pi) = 0$  for all non-zero integers  $l$  and for  $0 \leq n \leq m - 1$ . Differentiate (2

and in general we have

$$\sum_{k=-\infty}^{\infty} k^m \phi(x-k) = \sum_{n=0}^m \binom{m}{n} x^{m-n} (-1)^n \mu_n, \quad 0 \leq m \leq M-1. \quad (2)$$

If  $f \in L^2(\mathbf{R})$ , then  $\sum |s_k^j|^2 < \infty$ . Since the basis  $\phi_k^j, k \in \mathbf{Z}$  is orthonormal, it follows that

$$\|P_j f\|^2 = \sum_{-\infty}^{\infty} |s_k^j|^2.$$

We may also allow  $f$  to be a generalized function [3]. In this context, we take  $\phi_k^j, k \in \mathbf{Z}$  to be the test functions, and  $V_j$  to be the space of test functions. Then  $f$  is a continuous linear functional that assigns a unique real number  $(f, \phi_k^j)$  to each  $\phi_k^j \in V_j$ . If  $f$  is

We point out that in the inequality (2.46), in all practical cases the scale parameter  $j$  satisfies  $j \leq 0$ . Before proving the proposition we state and prove a combinatorial lemma.

**Lemma 2.2.5** *Let  $\{a_n\}$ ,  $\{b_n\}$ , and  $\{c_n\}$  be arbitrary sequences of length  $M$ , then we have*

$$\sum_{n=0}^{M-1} a_n \sum_{m=0}^{M-1-n} \binom{n+m}{n} b_m c_{n+m} = \sum_{m=0}^{M-1} c_m \sum_{n=0}^m \binom{m}{n} a_n b_{m-n}. \quad (2.47)$$

**Proof:** For convenience denote the left-hand side of (2.47) by l.h.s. Expanding the summation over  $n$  we have

$$\text{l.h.s.} = a_0 \sum_{m=0}^{M-1} \binom{0+m}{0} b_m c_{0+m} + \cdots + a_{M-1} \sum_{m=0}^0 \binom{M-1+m}{M-1} b_m c_{M-1+m}.$$

Now regroup these terms, factoring out in turn  $c_0$ ,  $c_1$ , etc. Since  $c_0$  appears only in the first term,  $c_1$  appears only in the first and second terms, etc., we obtain

$$\begin{aligned} \text{l.h.s.} &= c_0 \left\{ \binom{0}{0} a_0 b_0 \right\} + c_1 \left\{ \binom{1}{0} a_0 b_1 + \binom{1}{1} a_1 b_0 \right\} \\ &+ \cdots + c_{M-1} \left\{ \binom{M-1}{0} a_0 b_{M-1} + \binom{M-1}{1} a_1 b_{M-2} + \cdots + \binom{M-1}{M-1} a_{M-1} b_0 \right\}. \end{aligned}$$

This can evidently be written in compact notation as

$$\text{l.h.s.} = \sum_{m=0}^{M-1} c_m \sum_{n=0}^m \binom{m}{n} a_n b_{m-n},$$

which verifies (2.47).  $\square$

**Proof of the Proposition:** We first obtain an expression for the coefficient  $s_k^j$  in terms of the derivatives of  $f$ . Expanding  $f$  in a Taylor series about  $(2^j k)$  we have

$$f(x) = \sum_{m=0}^{M-1} \frac{f^{(m)}(2^j k)}{m!} (x - 2^j k)^m + \frac{f^{(M)}(\xi_k)}{M!} (x - 2^j k)^M$$

here  $\xi_k$  lies between  $x$  and  $(2^j k)$ . Using this expression we have

$$\begin{aligned} s_k^j &= 2^{-j/2} \int f(x) \phi(2^{-j} x - k) dx \\ &= 2^{-j/2} \sum_{m=0}^{M-1} \frac{f^{(m)}(2^j k)}{m!} 2^{mj} \int (2^{-j} x - k)^m \phi(2^{-j} x - k) dx + 2^{j/2} \varepsilon_k^j \\ &= 2^{j/2} \sum_{m=0}^{M-1} \frac{f^{(m)}(2^j k)}{m!} 2^{mj} \mu_m + 2^{j/2} \varepsilon_k^j \end{aligned}$$



so that (2.52) reduces to

$$(P_j f)(x) - E_j(x) = f(x).$$

This proves (2.45).

Now let us examine the error terms. Clearly

$$|E_j^1(x)| \leq C_0 \sup_k |\varepsilon_k^j|,$$

here we have used Lemma(2.2.1). Now consider

$$\begin{aligned} |\varepsilon_k^j| &\leq 2^{Mj} \int \frac{|f^{(M)}(\xi_k)|}{M!} |2^{-j}x - k|^M |\phi(2^{-j}x - k)| dx \\ &\leq 2^{(M+1)j} \sup_{\xi \in I_j(x)} \frac{|f^{(M)}(\xi)|}{M!} \int |x|^M |\phi(x)| dx \\ &\leq 2^{(M+1)j} C_M \sup_{\xi \in I_j(x)} \frac{|f^{(M)}(\xi)|}{M!} \end{aligned}$$

here we have used Lemma(2.2.2). Thus we have

$$|E_j^1(x)| \leq 2^{(M+1)j} C_0 C_M \sup_{\xi \in I_j(x)} \frac{|f^{(M)}(\xi)|}{M!} \quad (2.53)$$

Similarly we have

$$|E_j^2(x)| \leq 2^{Mj} C' C_M \sup_{\xi \in I_j(x)} \frac{|f^{(M)}(\xi)|}{M!}$$

here  $C' = \sum_{m=0}^{M-1} (|\mu_m|/m!) 2^{mj}$ . This proves (2.46).  $\square$

## 2.3 Multiresolution Approximation of Kernels

### 2.3.1 Kernels on $V_j$

In general, a kernel on  $V_j$  is an expression of the form

$$T_j(x, y) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} t_{m,n}^j \phi_m^j(x) \phi_n^j(y),$$

here the function  $\phi(x) \in V_0$  is the scaling function. In this thesis, we approximate kernels of the form  $K(x, y) = K(x - y)$ , and in this case the coefficients satisfy

$$t_{m,n}^j = t_{m-n}^j. \quad (2.54)$$

Therefore, for our purposes it is sufficient to view a kernel as an expression of the form

$$T_j(x, y) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} t_{m-n}^j \phi_m^j(x) \phi_n^j(y),$$

here the sequence  $\{t_n^j\}$  belongs to  $l^2(\mathbf{Z})$ . Thus, to build an approximation to a given kernel  $K(x - y)$  on the subspace  $V_j$ , it is necessary only to compute the appropriate coefficients. Conversely, the kernel  $T_j$  is completely determined once the coefficients  $\{t_n^j\}$  are known.

We note that (2.54) does not imply that  $T_j(x, y) = T_j(x - y)$ , i.e.  $T_j$  is not a convolutional kernel. However, we do have the identity

$$T_j(x + 2^j k, y + 2^j k) = T_j(x, y),$$

which shows that  $T_j$  is a "block convolution". To state this another way,  $T_j$  is a periodic function of period  $2^j$  in both  $x$  and  $y$ .



However, we also have

$$\begin{aligned}
(P_j K P_j f)(x) &= \int_{-\infty}^{\infty} T_j(x, y) f(y) dy \\
&= \int \sum_m \sum_n t_{m-n}^j \phi_m^j(x) \phi_n^j(y) f(y) dy \\
&= \sum_{m=-\infty}^{\infty} \phi_m^j(x) \sum_{n=-\infty}^{\infty} t_{m-n}^j \int \phi_n^j(y) f(y) dy \\
&= \sum_{m=-\infty}^{\infty} \phi_m^j(x) \sum_{n=-\infty}^{\infty} s_n^j t_{m-n}^j.
\end{aligned}$$

Equating these two expressions, we obtain

$$t_{m-n}^j = (K \phi_n^j, \phi_m^j) = \iint K(x-y) \phi_m^j(x) \phi_n^j(y) dy dx. \quad (2.55)$$

Using a change of variables and reversing the order of integration we can rewrite (2.55) as

$$t_n^j = \int_{-\infty}^{\infty} K(x) \Phi(2^{-j}x - n) dx, \quad (2.56)$$

here  $\Phi$  is the autocorrelation introduced in Section 2.1.3. Note also

*Suppose that  $K$  is at least  $M$  times  $c$*

Now use Proposition(2.2.1) to rewrite (2.62) as

$$\begin{aligned} T_j(x, y) - E_j(x, y) &= \sum_{m=0}^{M-1} \frac{K^{(m)}(x-y)}{m!} (-1)^m 2^{mj} \sum_{n=0}^m \binom{m}{n} (-1)^n \mu_{m-n} \mu_n \\ &= K(x-y) \end{aligned}$$

having also used Lemma(2.1.1), and Proposition(2.1.1). This proves (2.58).

Now consider the error terms. Taking  $m = M$  in (5.39), we have

$$\sup_{(k,l) \in \mathcal{K} \times \mathcal{L}} |\varepsilon_{k-l}^j| \leq 2^{(M+1)j} C_M \sup_{(\xi, \eta) \in R_j(x, y)} \frac{|K^{(M)}(\xi - \eta)|}{M!}.$$

Using this inequality, we have

$$\begin{aligned} &|E_j(x, y)| \\ &\leq \sup_{(k,l) \in \mathcal{K} \times \mathcal{L}} |\varepsilon_{k-l}^j| \left( \sum_k |\phi(2^{-j}x - k)| \right) \left( \sum_l |\phi(2^{-j}y - l)| \right) \\ &\quad + 2^{Mj} \sup_{(\xi, \eta) \in R_j(x, y)} \frac{|K^{(M)}(\xi - \eta)|}{M!} \sum_{n=0}^M \binom{M}{n} \\ &\quad \times \left( \sum_k |2^{-j}x - k|^{M-n} |\phi(2^{-j}x - k)| \right) \left( \sum_l |2^{-j}y - l|^n |\phi(2^{-j}y - l)| \right) \\ &\leq 2^{Mj} \sup_{(\xi, \eta) \in R_j(x, y)} \frac{|K^{(M)}(\xi - \eta)|}{M!} \left( C_1^2 + \sum_{n=0}^M \binom{M}{n} C_{M-n} C_n \right), \end{aligned}$$

which proves (2.59). The constants are those provided by Lemma(2.2.1).  $\square$

### 2.3.3 Trigonometric Expansion of a Kernel

The following theorem provides an efficient method for computing the value of  $T_j(x, y)$  at a given point  $(x, y)$ . As stated above (Section 2.3.1), the kernel  $T_j(x, y)$  is not a function of the difference  $(x - y)$  alone, a fact which makes it difficult to tabulate. However, it turns out that  $T_j$  may be represented by a sum of functions that depend only on  $(x - y)$ , and being functions of a single variable, are easily tabulated. The proof of this exploits the fact that  $T_j$  is periodic on a fixed diagonal  $x - y = \text{constant}$ .

The resulting series expansion (2.64) converges rapidly, and in our implementation we retain terms only for  $|n| \leq 3$ . This high rate of convergence follows from the rapid decay of the Fourier transform of the scaling function.

This result does not require the scaling function  $\phi$  to belong to an orthonormal system.

**Theorem 2.3.1** *Let  $\phi(x)$  be a scaling function for the subspace  $V_0$ , which is continuous and has a piecewise continuous derivative. Let  $T_j(x, y)$  be a kernel on  $V_j$ , which has the form*

$$T_j(x, y) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} t_{m-n}^j \phi_m^j(x) \phi_n^j(y), \quad (2.63)$$

where  $\sum |t_k^j|^2 < \infty$ . Then we have the identity,

$$2^j T_j(2^j x, 2^j y) = \sum_{n=-\infty}^{\infty} e^{in\pi(x+y)} I_n(x-y), \quad (2.64)$$

where

$$I_n(z) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-iz\xi} \hat{t}^j(\xi - n\pi) \hat{\Phi}_n(\xi) d\xi, \quad (2.65)$$

$$\hat{t}^j(\xi) = \sum_{k=-\infty}^{\infty} t_k^j e^{ik\xi}, \quad (2.66)$$

and

$$\hat{\Phi}_n(\xi) = \hat{\phi}(\xi - n\pi) \overline{\hat{\phi}(\xi + n\pi)}. \quad (2.67)$$

Furthermore, for each  $(x, y) \in \mathbf{R}^2$ , the right-hand-side of (2.64) converges uniformly to  $2^j T_j(2^j x, 2^j y)$ .

**Example:** In order to illustrate the decay of the functions  $\hat{\Phi}_n(\xi)$ , assume that  $\phi(x)$  is the central B-spline of degree  $(2m - 1)$ . Then we have

$$\hat{\Phi}_n(\xi) = \left[ \frac{\sin\left(\frac{\xi}{2} + \frac{n\pi}{2}\right)}{\frac{\xi}{2} + \frac{n\pi}{2}} \right]^{2m} \left[ \frac{\sin\left(\frac{\xi}{2} - \frac{n\pi}{2}\right)}{\frac{\xi}{2} - \frac{n\pi}{2}} \right]^{2m}$$

which obviously decays rapidly as  $|n| \rightarrow \infty$ .

**Proof of the Theorem:**



Alternatively, we can write

$$\begin{aligned}
2^j T_j(2^j x, 2^j y) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\xi(x-y)} \hat{t}^j(\xi) |\hat{\phi}(\xi)|^2 d\xi \\
&+ \sum_{n=1}^{\infty} \frac{1}{\pi} \int_{-\infty}^{\infty} e^{-i\xi(x-y)} t^j(\xi - n\pi) \operatorname{Re} \{ e^{in\pi(x+y)} \hat{\Phi}_n(\xi) \} d\xi. \quad (2.73)
\end{aligned}$$

When the functions  $\hat{\Phi}_n(\xi)$  are real, this reduces to

$$\begin{aligned}
2^j T_j(2^j x, 2^j y) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\xi(x-y)} \hat{t}^j(\xi) |\hat{\phi}(\xi)|^2 d\xi \\
&+ \sum_{n=1}^{\infty} \cos[n\pi(x+y)] \cdot \frac{1}{\pi} \int_{-\infty}^{\infty} e^{-i\xi(x-y)} t^j(\xi - n\pi) \hat{\Phi}_n(\xi) d\xi. \quad (2.74)
\end{aligned}$$

## 2.4 Spline MRAs

An important class of multiresolution analyses use splines as a starting point (see e.g. [5] or [20]). In this thesis, we restrict our attention to the central B-splines of odd degree, though splines of even degree could also be used. Integer translates of these functions form a Riesz basis.

We denote by  $\beta^{(M-1)}(x)$  the spline that is piecewise polynomial of degree  $(M-1)$ , for  $M = 2, 4, \dots$ . By way of example, the lowest order case, corresponding to  $M = 2$ , is the well-known “hat function”,

$$\beta^{(1)}(x) = \begin{cases} 1 - |x|, & |x| < 1 \\ 0, & |x| \geq 1. \end{cases} \quad (2.75)$$

These functions are compactly supported,

**f** **A d f B**

here  $\beta^{(0)}(x)$  is the characteristic function of the interval  $[-1/2, 1/2)$ . (Here we allow  $m$  to be any non-negative integer.) We can also write

$$\beta^{(m)}(x) = \int_{-1/2}^{1/2} \beta^{(m-1)}(x-t) dt, \quad m \geq 1.$$

Using the fact that  $\beta^{(m)}$  is an  $(m+1)$ -fold convolution

### 2.4.1 The Battle-Lemarié Scaling Function

The scaling function for the orthonormal system in a spline MRA is known as the Battle-Lemarié scaling function (see e.g. [8, pp.146-152]). This scaling function is the result of applying the orthogonalization procedure (2.7) to the B-spline. The Battle-Lemarié function is thus defined in the Fourier domain by the equation

$$\hat{\phi}^{(M-1)}(\xi) = \prod_{k=1}^M \frac{1 + e^{-i\xi} + \dots + e^{-i(k-1)\xi}}{k}$$





Using Poisson's summation formula, the relationship (2

Let  $M$  be an even, positive integer and let  $(M - 1)$  be the degree of the B-spline  $\beta$ . Construct two sets of numbers  $\{q_m\}_{m=0}^{M-1}$  and  $\{Q_m\}_{m=0}^{2M-1}$  according to the formulae

$$\sum_{n=0}^m \binom{m}{n} (-1)^n q_{m-n} \mu_n = \begin{cases} 1, & m = 0 \\ 0, & m > 0 \end{cases} \quad \text{for } 0 \leq m \leq M - 1 \quad (2.97)$$

and

$$\sum_{n=0}^m \binom{m}{n} (-1)^n Q_{m-n} \mathcal{M}_n = \begin{cases} 1, & m = 0 \\ 0, & m > 0 \end{cases} \quad \text{for } 0 \leq m \leq 2M -$$

where

$$|E_j(x)| \leq 2^{Mj} C \sup_{\xi \in I_j(x)} \frac{|f^{(M)}(\xi)|}{M!}. \quad (2.103)$$

The constant  $C$  depends on  $\beta$  but not on  $f$ .

**Proof:** Let  $x_0$  be an arbitrary real number. Expand  $f$  in a Taylor series about  $x_0$  to obtain the expression for the  $m$ th derivative,

$$f^{(m)}(x) = \sum_{n=0}^{M-1-m} \frac{f^{(n+m)}(x_0)}{n!} (x - x_0)^n + \frac{f^{(M)}(\xi_m)}{M!} (x - x_0)^M,$$

here  $0 \leq m \leq M - 1$ , and  $\xi_m$  lies between  $x$  and  $x_0$ . Set  $x = 2^j k$  to obtain

$$f^{(m)}(2^j k) = \sum_{n=0}^{M-1-m} \frac{f^{(n+m)}(x_0)}{n!} (2^j k - x_0)^n + \frac{f^{(M)}(\xi_{m,k})}{M!} (2^j k - x_0)^M,$$

here  $\xi_{m,k}$  lies between  $x_0$  and  $(2^j k)$  for each  $m$ . Now use this expression together with (2.99) to write

$$\begin{aligned} (P_j f)(x_0) &= 2^{-j/2} \sum_k s_k^j \beta(2^{-j} x_0 - k) \\ &= \sum_k \beta(2^{-j} x_0 - k) \sum_{m=0}^{M-1} \frac{f^{(m)}(2^j k)}{m!} 2^{mj} q_m \\ &= \sum_k \beta(2^{-j} x_0 - k) \sum_{m=0}^{M-1} \frac{q_m}{m!} \left\{ \sum_{n=0}^{M-1-m} \frac{f^{(n+m)}(x_0)}{n!} (2^j k - x_0)^n \right. \\ &\quad \left. + \frac{f^{(M)}(\xi_{m,k})}{M!} (2^j k - x_0)^M \right\} \\ &= \sum_{m=0}^{M-1} q_m \sum_{n=0}^{M-1-m} \frac{f^{(n+m)}(x_0)}{m! n!} 2^{(m+n)j} (-1)^n \\ &\quad \times \sum_k (2^{-j} x_0 - k)^n \beta(2^{-j} x_0 - k) + E_j(x_0), \end{aligned} \quad (2.104)$$

here we have put

$$E_j(x) = \sum_{m=0}^{M-1} \frac{q_m}{m!} \sum_k \frac{f^{(M)}(\xi_{m,k})}{M!} (2^j k - x)^M \beta(2^{-j} x - k). \quad (2.105)$$

Continuing from (2.104), and using the identity (2.80), we have

$$\begin{aligned} (P_j f)(x_0) - E_j(x_0) &= \sum_{m=0}^{M-1} q_m \sum_{n=0}^{M-1-m} \frac{f^{(n+m)}(x_0)}{m! n!} 2^{(m+n)j} (-1)^n \mu_n \\ &= \sum_{m=0}^{M-1} q_m \sum_{n=0}^{M-1-m} \binom{n+m}{m} \frac{f^{(n+m)}(x_0)}{(n+m)!} 2^{(m+n)j} (-1)^n \mu_n. \end{aligned}$$

No use (2.47) to transform the right-hand side of this equation, thus obtaining

$$\begin{aligned} (P_j f)(x_0) - E_j(x_0) &= \sum_{m=0}^{M-1} \frac{f^{(m)}(x_0)}{m!} 2^{mj} \sum_{n=0}^m \binom{m}{n} (-1)^n q_{m-n} \mu_n \\ &= f(x_0), \end{aligned}$$

here we have used (2.97). This proves (2.102).

Finally, we observe that, since  $\beta$  is compactly supported, there is a constant  $C_M$  such that

$$\sum_{-\infty}^{\infty} |x - k|^M |\beta(x - k)| \leq C_M,$$

by Lemma(2.2.1). Thus, from (2.105) we have

$$\begin{aligned} |E_j(x)| &\leq \left( \sum_{m=0}^{M-1} \frac{|q_m|}{m!} 2^{mj} \right) 2^{Mj} \sum_k |2^{-j}x - k|^M |\beta(2^{-j}x - k)| \frac{|f^{(M)}(\xi_{m,k})|}{M!} \\ &\leq 2^{Mj} C' C_M \sup_{\xi \in I_j(x)} \frac{|f^{(M)}(\xi)|}{M!}, \end{aligned}$$

here  $C' = \sum_{m=0}^{M-1} 2^{mj} (|q_m|/m!)$ . This verifies (2.103).  $\square$

**Proposition 2.4.2** *Let  $\beta$  be the central B-spline of degree  $(M - 1)$ , where  $M$  is an even positive integer. Let  $T_j = P_j K P_j$  denote the projection of a kernel  $K$  onto the subspace  $V_j$ , given by*

$$T_j(x, y) = \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} t_{k-l}^j \beta_k^j(x) \beta_l^j(y) \quad (2.106)$$

where the coefficients are given by (2.100). For a given point  $(x, y) \in \mathbf{R}^2$ , let  $R_j(x, y)$  be the rectangle formed by the union of the supports of all basis functions which are non-zero at  $(x, y)$ . Thus, if

$$I_j(x) = \bigcup_{k \in \mathcal{K}} \text{supp}(\beta_k^j), \quad \mathcal{K} = \{k \in \mathbf{Z} | \beta_k^j(x) \neq 0\}$$

and

$$I_j(y) = \bigcup_{l \in \mathcal{L}} \text{supp}(\beta_l^j), \quad \mathcal{L} = \{l \in \mathbf{Z} | \beta_l^j(y) \neq 0\}$$

then

$$R_j(x, y) = I_j(x) \times I_j(y).$$

Suppose that  $K$  is at least  $M$  times continuously differentiable on  $R_j(x, y)$ . Then we have

$$T_j(x, y) = K(x - y) + E_j(x, y), \quad (2.107)$$

where

$$|E_j(x, y)| \leq 2^{Mj} C \sup_{(\xi, \eta) \in R_j(x, y)} \frac{|K^{(M)}(\xi - \eta)|}{(M)!}. \quad (2.108)$$

The constant  $C$  depends on  $\beta$  but not on  $K$ .

The proof of this proposition is similar t

which follows from (2.92). Comparison of this expression with (2.81) shows that

$$\hat{A}(\xi) = |\hat{\phi}(\xi)|^2$$

where  $\phi$  is the Battle-Lemarié scaling function. Thus the correlation function  $A$  is equal to the autocorrelation of the Battle-Lemarié scaling function almost everywhere, which by Proposition(2.1.1) must have vanishing moments. Let  $\mathcal{A}_m$  denote the  $m$ th moment of  $A$ . Then we have

$$\mathcal{A}_m = \begin{cases} 1, & m = 0 \\ 0, & m > 0 \end{cases}$$

for  $0 \leq m \leq 2M - 1$ , and as in Lemma(2.1.1) we have

$$\mathcal{A}_m = \sum_{n=0}^m \binom{m}{n} (-1)^n q_{m-n} \mu_n.$$

Since the moments of the B-spline  $\{\mu_n\}$  are easy to compute, (use the recursive formula in equation 2.22)

# Chapter 3

## The Fast Summation Algorithm in One Dimension

In this chapter we describe our approach for problems in one dimension. Our approach in higher dimensions is similar. Indeed, to develop an algorithm in two dimensions, the only additional machinery used is singular value decomposition of the coefficient matrix, but this will be discussed in Chapter(4).

### 3.1 General Description

1. Our goal is to compute the numbers  $\{g_m\}$ , here

$$g_m = \sum_{\substack{n=1 \\ n \neq m}}^N K(x_m - x_n) f_n, \quad 1 \leq m \leq N. \quad (3.1)$$

We assume that the kernel  $K$  is singular on the line  $x - y = 0$ , i.e.

$$|K(x - y)| \rightarrow \infty \quad \text{as} \quad (x - y) \rightarrow 0,$$

but is at least  $M$  times continuously differentiable on any region that does not contain the line  $x = y$ . Moreover, we assume that there is a “band width”  $B$  such that the  $M$ th derivative is uniformly bounded outside the band  $|x - y| < B$ , i.e.

$$|K^{(M)}(x - y)| \leq C \quad \text{for} \quad |x - y| \geq B. \quad (3.2)$$

2. We choose a level of refinement ( $j \leq 0$ ), a multiresolution analysis with  $M$  vanishing moments, and construct the projection of the kernel onto the subspace  $V_j$ , given by  $\mathcal{E}$



As discussed in Chapter(2) this construction requires only the computation of the coefficients  $\{t_n^j\}$ , given by

$$t_n^j = \int_{-\infty}^{\infty} K(x)\Phi(2^{-j}x - n) dx, \quad n \in \mathbf{Z}$$

here  $\Phi$  is the autocorrelation of the scaling function  $\phi$ . This can be done ahead of time and the coefficients  $\{t_n^j\}$  are then stored in memory. This portion of the computation is part of the initialization.

**3.** Using Proposition(2.3.1) together with (3.2) we have the estimate

$$|K(x - y) - T_j(x, y)| \leq \epsilon \quad \text{for} \quad |x - y| \geq 2^j B, \quad (3.4)$$

for any  $\epsilon > 0$ , provided that  $M$  and  $j \leq 0$  have been chosen so that  $C(2^{Mj}/M!) < \epsilon$ . (There is some abuse of notation here, since the constants  $C$  and  $B$  are not necessarily identical to the co

and

$$s_l^j = \sum_{n=1}^N f_n \phi_l^j(x_n). \quad (3.9)$$

small, and hence points (

**2.** The number of vanishing moments  $M$  corresponds to a B-spline of degree  $(2m - 1)$ . More precisely, we have  $M - 1 = 2m - 1$ , so that  $M$  must be an even, positive integer. Once this parameter and the level of refinement  $j \leq 0$  have been chosen, the projection of the kernel  $K$  is

$$T_j(x, y) = \sum_{k=0}^{J-1} \sum_{l=0}^{J-1} t_{k-l}^j \beta_k^j(x) \beta_l^j(y), \quad (3.15)$$

here  $J = 2^{-j}$ , and  $\beta$  denotes the B-spline of degree  $(2m - 1)$ . The coefficients  $\{t_n^j\}$  for  $|n| \leq (J - 1)$  are computed using the formula (2.100).

**3.** Note that, in anticipation of

**6.** Having obtained the coefficients (3.18) we can now evaluate the expansion

$$g^j(x) = \sum_{k=0}^{J-1} c_k x^k$$



**Step Procedure**

**Complexit**





and then e

$N$	$T_{LF}$	$T_{HF}$	$T_{tot}$	$T_{dir}$	$E_2$	$E_\infty$
64	0.0036	0.0037	0.0073	0.0077	0.46860E-05	0.35852E-05
128	0.0066	0.0079	0.0145	0.0278	0.41383E-05	0.47034E-05
256	0.0138	0.0155	0.0293	0.1044	0.38780E-05	0.42643E-05
512	0.0264	0.0300	0.0564	0.4042	0.36356E-05	0.43642E-05
1024	0.0552	0.0591	0.1143	1.5946	0.33201E-05	0.33570E-05
2048	0.1089	0.1175	0.2264	6.3151	0.31335E-05	0.33471E-05
4096	0.2379	0.2351	0.4731	25.2104	0.33210E-05	0.31553E-05

**T**

$N$	$T_{LF}$	$T_{HF}$	$T_{tot}$	$T_{dir}$	$E_2$	$E_\infty$
64	0.0138	0.0130	0.0268	0.0086	0.50929E-14	0.26622E-14
128	0.0261	0.0260	0.0521	0.0318	0.23669E-14	0.16785E-14
256	0.0525	0.0477	0.1002	0.1244	0.43058E-14	0.18982E-14
512	0.1111	0.0925	0.2036	0.4910	0.85681E-14	0.43438E-14
1024	0.2344	0.1770	0.4114	2.0113	0.78821E-14	0.25543E-14
2048	0.5288	0.3593	0.8881	8.0242	0.91355E-14	0.27125E-14
4096	1.0738	0.7384	1.8122	32.1545	0.11375E-13	0.66191E-14

Table 3.3: Implementation in one dimension using B-splines of degree 11, break-even at about 220 particles.

can then be computed with the standard FFT. In order to determine the coefficients  $\{g_m\}$ , we invert (3.31) to get

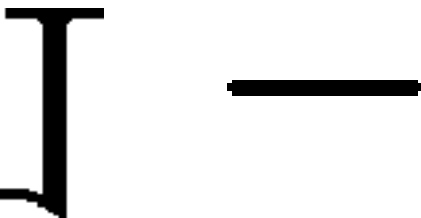
$$g_m = \frac{1}{N} \sum_{j=0}^{N-1} \hat{f}_j e^{-2\pi i m j / N}.$$

Next substitute expression (3.29) for  $\hat{f}_j$  to get

$$\begin{aligned} g_m &= \frac{1}{N} \sum_{j=0}^{N-1} e^{-2\pi i m j / N} \sum_{n=0}^{N-1} f_n e^{2\pi i j x_n} \\ &= \sum_{n=0}^{N-1} f_n \frac{1}{N} \sum_{j=0}^{N-1} e^{-2\pi i j (m/N - x_n)}, \end{aligned} \quad (3.32)$$

here  $f_n = f(x_n)$ . Now we have

$$\begin{aligned} \sum_{j=0}^{N-1} e^{-2\pi i j (m/N - x_n)} &= \frac{1 - e^{-2\pi i (m/N - x_n) N}}{1 - e^{-2\pi i (m/N - x_n)}} \\ &= -2e^{i\pi N x_n} \frac{\sin(\pi N (m/N - x_n))}{\sin(\pi (m/N - x_n))} \end{aligned}$$





Now, in order to find an explicit representation for  $\tilde{T}_j$ , we proceed as follows. Assume that we have constructed  $T_j$  and  $T_{j+1}$ . Then we have

$$T_j(x, y) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} t_{m-n}^j \phi_m^j(x) \phi_n^j(y), \quad (3.41)$$

and

$$T_{j+1}(x, y) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} t_{m-n}^{j+1} \phi_m^{j+1}(x) \phi_n^{j+1}(y). \quad (3.42)$$

In order to express  $T_{j+1}$  in terms of the basis functions  $\phi_n^j, n \in \mathbf{Z}$  in  $V_j$ , we use the two-scale difference equation (2.8) satisfied by the scaling function  $\phi(x)$ , which takes the general form

$$\phi_k^{j+1}(x) = \sum_l h_{l-2k} \phi_l^j(x). \quad (3.43)$$

Using (3.43) in (3.42), we have

$$T_{j+1}(x, y) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty}$$

$V_j, \dots, V_{j+n}$ . This is done as follows. Recall that (see equation (3.9)) the coefficients  $\{s_i^j\}$  that represent the particle distribution on  $V_j$  are given by

## chapter 4

# The Fast Summation Algorithm in Higher Dimensions

In this chapter, we explain how to extend our one-dimensional scheme to higher dimensions. The algorithm has been implemented in two dimensions, and we give details of this and also present some numerical results. As mentioned above, there is little here beyond the use of vector notation that is not completely analogous to the one-dimensional case, except for singular value decomposition of the coefficient matrix (this matrix is defi





## 4.2 The Fast Summation Algorithm in Two Dimensions

1. Our goal is to compute

$$g(x_m, y_m) = \sum_{i=0}^N$$

2.3.3. Since we are using central B-splines as basis functions, the functions  $\hat{\Phi}_n(\xi)$  are real. In this case, we can write

$$4^j T_j(2^j x, 2^j y, 2^j x', 2^j y')$$

$$= I_{0,0}(z, z') + 2 \sum_{n=1}^{\infty} \cos(n\pi w') I_{0,n}(z, z') + 2 \sum_{m=1}^{\infty} \cos(m\pi w) I_{m,0}(z, z')$$

Defining

$$\begin{aligned} U_m^{(r)}(z) &= \sum_k u_k^{(r)} \Phi_m(z - k) \\ V_n^{(r)}(z') &= \sum_l v_l^{(r)} \Phi_n(z' - l), \end{aligned}$$

we can express  $I_{m,n}$  in the form

$$I_{m,n}(z, z') = \sum_{r=1}^R \sigma_r U_m^{(r)}(z) V_n^{(r)}(z'). \quad (4.13)$$

5. Substituting (4.13) into (4.8), we obtain our final expression for the trigonometric expansion of the kernel,

$$\begin{aligned} 4^j T_j(2^j x, 2^j y, 2^j x', 2^j y') &= \sum_{r=1}^R \sigma_r \left\{ U_0^{(r)}(z) + 2 \sum_{m=1}^{\infty} \cos(m\pi w) U_m^{(r)}(z) \right\} \\ &\times \left\{ V_0^{(r)}(z') + 2 \sum_{n=1}^{\infty} \cos(n\pi w') V_n^{(r)}(z') \right\}. \quad (4.14) \end{aligned}$$

Once the functions  $U_m^{(r)}(z)$  and  $V_n^{(r)}(z')$  have been tabulated, the cost of eval-

The errors are computed according to the following formulae. Suppose that  $\mathbf{x}$  is the “exact”  $N$ -length vector, and  $\tilde{\mathbf{x}}$  is the approximation. Then we compute the relative errors

$$E = \frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\|\mathbf{x}\|},$$

here

$$\|\mathbf{x}\|_2^2 = \frac{1}{N} \sum_{i=1}^N |x_i|^2, \quad \|\mathbf{x}\|_\infty = \max_{1 \leq i \leq N} |x_i|.$$

The timings were done on 10/30/96 using a Sun Sparc-20 workstation.

$N$	$T_{\text{LF}}$	$T_{\text{HF}}$	$T_{\text{tot}}$	$T_{\text{dir}}$	$E_2$	$E_\infty$
64	0.0920	0.0435	0.1355	0.0124		

21991 || x

## chapter 5

# Regularization of Singular Operators

One often encounters discrete sums that do not have a direct analogue as an integral operator. For example, the expression

$$(Kf)(x) = \int_{-\infty}^{\infty} \frac{f(y)}{|x-y|^2} dy \quad (5.1)$$

requires special interpretation as an operator. By contrast, the discrete sum

$$g(x_m) = \sum_{\substack{n=1 \\ n \neq m}}^N \frac{f(x_n)}{|x_m - x_n|^2}, \quad 1 \leq m \leq N \quad (5.2)$$

presents no difficulties. In our approach to the computation of such sums, we construct kernels  $T_j : V_j \rightarrow V_j, j \in \mathbb{Z}$  which are approximations of the kernel functions that appear in the summation problem. However, it is clear that the same approximation  $T_j$  may be used to provide a definition of the corresponding integral operator.

Thus, for example, if we have constructed a kernel  $T_j$  such that the sum

$$g^j(x_m) = \sum_{\substack{n=1 \\ n \neq m}}^N T_j(x_m, x_n) f(x_n), \quad 1 \leq m \leq N \quad (5.3)$$

## 5.1 Preliminary Considerations

In order to construct a kernel  $T_j$  that represents a linear operator  $K$  on the subspace  $V_j$  of a multiresolution analysis, it is

For operators satisfying these conditions, the projections of the corresponding kernels  $T_j : V_j \rightarrow V_j$  have the form

$$T_j(x, y) = 2^{-j(1+\alpha)} T(2^{-j}x, 2^{-j}y), \quad (5.12)$$

for any  $j \in \mathbb{Z}$ , here

$$T(x, y) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} t_{m-n} \phi(x-m) \phi(y-n), \quad (5.13)$$

and the coefficients are given by the functional

$$t_n = (\phi_n^0, K\phi_0^0), \quad (5.14)$$

here

$$(\phi_n^0, K\phi_0^0) = \int_{-\infty}^{\infty} \phi(x-n)(K\phi)(x) dx \quad (5.15)$$

whenever the right-hand side of (5.15) exists.

As examples, we consider below the following integral operators with algebraic singularities

$$(Kf)(x) = \int_{-\infty}^{\infty} \frac{f(y)}{(x-y)^{1+\alpha}} dy, \quad \alpha \geq -1 \quad (5.16)$$

and

$$(Kf)(x) = \int_{-\infty}^{\infty} \frac{f(y)}{|x-y|^{1+\alpha}} dy, \quad \alpha \geq -1 \quad (5.17)$$

For  $\alpha = 0$ , the expression (5.15) defines a bounded operator on  $L^2(\mathbf{R})$ , provided that we consider the principle value at  $x = y$ . When suitably scaled, this example is known as the Hilbert transform. However, for most values of  $\alpha$ , the operators (5.16) and (5.17) are not bounded on  $L^2(\mathbf{R})$ . It has been shown in [2] that the derivative operators  $(d/dx)^\alpha$ , for  $\alpha = 1, 2, \dots$  also satisfy the conditions stated above, and have representations of the form (5.12).

## 5.2 Classical Regularization of Divergent Integrals

Our task is to give a meaning to the functional (5.14) when the integral (5.15) is divergent. To this end, we first recall how such problems have been addressed up to now.

As an example, consider the expression

$$\int_{-\infty}^{\infty} \frac{\phi(x)}{x} dx, \quad (5.18)$$

here  $\phi$  is an infinitely differentiable function with compact support,  $\phi \in C_0^\infty(\mathbf{R})$ . This integral converges for all test functions  $\phi$  that vanish in a neighborhood of the origin. However, the integral diverges if  $\phi(0) \neq 0$ . We now ask whether it is possible to define a functional  $(x^{-1}, \phi)$  such that, for all test functions  $\phi$  that vanish in a neighborhood of zero, the functional has the value given by (5.18). The functional  $(x^{-1}, \phi)$  is then called a regularization of the divergent integral (5.18) (see e.g. [13, pp.10-12]).

The functional

$$(x^{-1}, \phi) = \int_{-\infty}^{-\epsilon} \frac{\phi(x)}{x} dx + \int_{-\epsilon}^{\epsilon} \frac{\phi(x) - \phi(0)}{x} dx + \int_{\epsilon}^{\infty} \frac{\phi(x)}{x} dx, \quad (5.19)$$

where  $\epsilon$  is any positive real number, obviously reduces to (5.18) if  $\phi(0) = 0$ . Moreover, since  $\phi(x) - \phi(0) \sim x\phi'(0)$  as  $x \rightarrow 0$ , it



In the following section, we present a method for regularization of the integral (5.15), thus providing a meaning to the functional (5.14), which utilizes the multiresolution approach. For integral operators with algebraic singularities, our approach produces the same results as the classical regularization method, with the additional benefit of a practical scheme for computation. Furthermore, it appears that our approach may also be applied to classes of operators with more general types of singularities.

## 5.3 A Multiresolution Approach to Regularization

### 5.3.1 Choice of the Scaling Function

Throughout this chapter, we limit our consideration to a specific family of MRAs, namely, those belonging to the compactly supported scaling functions constructed by I. Daubechies [7]. These scaling functions and their autocorrelations were introduced in Section 2.1.4.

We recall that for the MRA with  $M$  vanishing moments, the autocorrelation  $\Phi(x)$  is supported on the interval  $[1 - 2M, 2M - 1]$ , and also that the coefficients  $\{a_m\}$  in the two-scale difference equation (2.28) for  $\Phi(x)$  are given explicitly in (2.29).

### 5.3.2 Two-Scale Difference Equation for the Coefficients

In this section we derive the following necessary condition on the functional (5.14),

$$2^{-n} t_n = t_{2n} + \frac{1}{2} \sum_{m=1}^M a_{2m-1} [t_{2n-2m+1} + t_{2n-1+2m}]. \quad (5.24)$$

We refer to (5.24) as the two-scale difference equation. This equation is the tool that we use

obtained by setting  $j = 0$  in (5.11). The scaling function  $\phi(x)$  satisfies the two-scale difference equation

$$\phi(x) = \sqrt{2} \sum_{k=0}^{2M-1} h_k \phi(2x - k),$$

which can be written as

$$\phi_n^{(0)}(x) =$$

for the regularization of such operators. We show its consistency with the classical definition (see Section 5

We are not in a position to give a constructive definition of the multiresolution regularization of the operator  $K$ .

**Definition 5**



### 5.3.4 Classical vs Multiresolution Regularization

Consider the integral operator

$$(Kf)(x) = \int_{-\infty}^{\infty} \frac{f(y)}{(x-y)^{1+\alpha}} dy,$$

here  $\alpha = 0, 1, 2, \dots$  as an example. Projection of this operator onto the subspace  $V_0$  of the MRA with  $M$  vanishing moments (see Section 5.3.1) requires evaluation of the integral

$$t_n = \int_{-\infty}^{\infty} \phi(x-n)(K\phi)(x) dx,$$

which can also be written as

$$t_n = \int_{-\infty}^{\infty} \frac{\Phi(x-n)}{x^{1+\alpha}} dx, \quad (5.31)$$

where  $\Phi(x)$  is the autocorrelation of  $\phi(x)$  (see equation (2.56)). The support of  $\Phi(x)$  is the closed interval  $[1-2M, 2M-1]$ . Hence the integral (5.31) is well defined whenever  $|n| \geq 2M$ , since for these values of  $n$ , the support of  $\Phi(x-n)$  does not contain the origin.

We consider a regularization on  $\mathbb{R}^d$

and the regularization of this integral is the functional

$$t_n = \left( x^{-1-}, \Phi(x - n) \right)$$

Now, since  $a_{-m} = a_m$ , it follows that

$$\int_0^\infty \frac{dx}{x^{1+}} \frac{1}{2} \sum_m a_m \{ \Phi(x - 2n - m) - \Phi(x - 2n + m) \} = 0.$$

Therefore, we have

$$\begin{aligned} 2^{-n} t_n &= \frac{1}{2} \sum_m a_m \int_0^\infty \frac{dx}{x^{1+}} [\Phi(x - 2n + m) - \Phi(x + 2n - m)] \\ &\quad - 2 \sum_{k=0}^{(-1)/2} \frac{\Phi^{(2k)}(2n - m)}{(2k)!} x^{2k} \\ &= \frac{1}{2} \sum_m a_m t_{2n-m} = \frac{1}{2} \sum_m a_m t_{2n+m}. \end{aligned}$$

As this result is valid for all  $n \in \mathbf{Z}$ , the two-scale difference equation (5.24) is satisfied. The procedure for (5.35) is identical.  $\square$

**Proposition 5.3.1** *The classical regularization and the multiresolution regularization of (5.31) produce identical results.*

**Proof:** The coefficients  $t_n$  for  $|n| \geq 2M$  computed in Steps 1 and 2 of the algorithm of Section 5.3 agree with the integral expression (5.31)



It is shown in [2] that eigenvectors of  $A$  belonging to the eigenvalues  $2^{-\alpha}$  are composed of the values of the  $\alpha$ th derivative of  $\Phi(x)$ , taken at the integers. That is, if

$$v = \{\Phi^{(\alpha)}(1 - 2M), \dots, \Phi^{(\alpha)}(2M - 1)\},$$

then  $Av = 2^{-\alpha} v$ . Furthermore, the  $\alpha$ th derivative  $\Phi^{(\alpha)}(x)$  exists and is continuous if and only if  $2^{-\alpha}$  is an eigenvalue of  $A$ , and is nondegenerate.

Hence, to prove the proposition, it is necessary and sufficient to show that

$$\sum_{n=1-2M}^{2M-1} t_n \Phi^{(\alpha)}(n) = 0, \quad (5.36)$$

here the coefficients  $t_n$  are given by (5.33) or (5.35).

Now consider the following. Since  $\Phi(-x) = \Phi(x)$ , it follows that if  $\alpha$  is even, then  $\Phi^{(\alpha)}(-x) = \Phi^{(\alpha)}(x)$ , and if  $\alpha$  is odd, then  $\Phi^{(\alpha)}(-x) = -\Phi^{(\alpha)}(x)$ . Now, from (5.31) it follows that if  $\alpha$  is even, then  $t_{-n} = -t_n$ , and if  $\alpha$  is odd, then  $t_{-n} = t_n$ . Thus (5.36) is always satisfied.  $\square$

**Remark:** The fact that the classical regularization and the multiresolution regularization of (5.31) produce identical results proves that the limit of the regularized kernel  $T_j$ , as  $j \rightarrow -\infty$ , is independent of the basis chosen, at least in those cases in which both methods are applicable.

then  $t_{-}$

digits of accuracy. By contrast, the column marked “MRA” is correct to the accuracy  $\epsilon$  chosen in Step 1 of the algorithm.

<b>n</b>	<b>Classical</b>	<b>MRA</b>
0	-5.471	-5.508
1	2.359	2.375
2	-0.058	-0.059
3	0.150	0.152
4	0.064	0.064
5	0.040	0.041

### 5.3.5 Asymptotic Condition for Integral Operators

For integral operators, the coefficients  $t_n$ ,  $n \in \mathbf{Z}$  are computed according to the formula

$$t_n^j = \int_{-\infty}^{\infty} K(x) \Phi(2^{-j}x - n) dx,$$

here  $\Phi(x)$

With the change of variable  $y = 2^{-j}x - n$  this reduces to

$$\begin{aligned} t_n^j &= \sum_{l=0}^{m-1} \frac{K^{(l)}(2^j n)}{l!} 2^{(l+1)j} \int_{-\infty}^{\infty} y^l \Phi(y) dy + \varepsilon_n^j \\ &= 2^j K(2^j n) + \varepsilon_n^j, \end{aligned}$$

which follows from Proposition (2.1.1), since  $m - 1 \leq 2M - 1$ .

Now let us consider the error term (5.4) by using the Taylor expansion of  $\Phi$  at  $2^j n$ . We have

here  $t_n, n \in \mathbf{Z}$  are the coefficients that satisfy the two-scale difference equation (5.24). Recall the definition of the trigonometric series  $M_0(\xi)$  from equation (2.17),

$$M_0(\xi) = \frac{1}{4} \sum_{-\infty}^{\infty} a_m e^{im\xi},$$

which for the MRAs under consideration (see Section 5.3.1) has the form

$$M_0(\xi) = \frac{1}{2} + \frac{1}{4} \sum_{m=1}^M a_{2m-1} e^{im\xi}$$



But  $\sup |M_0(\xi)|^2 = 1$ , so we have

$$\|M_0^* g\|^2 \leq 4\|g\|^2,$$

which implies that  $\|M_0^*\| \leq 2$ .

Next, we make use of the fact that  $M_0(0) = 1$ . Define the sequence of functions  $g_n(\xi) = \sqrt{n}$  if  $|\xi| < 1/n$ , 0 otherwise. Then we have

$$\begin{aligned} \|M_0^* g_n\|^2 &= \int_{-\pi}^{\pi} |(M_0^* g_n)(\xi)|^2 d\xi \\ &= n \int_{-1/2n}^{1/2n} |2M_0(\xi)|^2 d\xi, \end{aligned}$$

and by the continuity of  $M_0$  we have

$$\|M_0^* g_n\|^2 \rightarrow |2M_0(0)|^2 = 4,$$

**Proposition 5.4.3** *Let  $K$  be a linear, homogeneous operator that commutes with translation. If the quantities*

$$t_n = \int_{-\infty}^{\infty} \phi(x-n)(K\phi)(x) dx$$

*are well-defined for every integer  $n$ , then the series  $\hat{t}(\xi) = \sum t_n e^{in\xi}$  satisfies the eigenvalue equation*

$$(M_0 \hat{t})(\xi) = 2^{-} \hat{t}(\xi).$$

Thus, the sequence  $t_n, n \in \mathbf{Z}$  may be identified with a trigonometric series  $\hat{t}(\xi)$ , which is an eigenvector of the operator  $M_0$ . The question therefore arises whether or not the regularization produced by the algorithm of Section 5.3.3 is an eigenvector of  $M_0$ .

**Proposition 5.4.4** *Let  $K$  be a linear operator that is homogeneous of degree  $\alpha$  and commutes with translation. Let  $t_n, n \in \mathbf{Z}$  be the regularization computed according to the algorithm of Section 5.3.3. Let  $\hat{t}(\xi)$  be the formal trigonometric series  $\sum t_n e^{in\xi}$ . If  $2^{-}$  is not an eigenvalue of the matrix  $A$ , then  $\hat{t}$  satisfies the eigenvalue equation*

$$(M_0 \hat{t})(\xi) = 2^{-} \hat{t}(\xi).$$

*If  $2^{-}$  is an eigenvalue of  $A$ , then  $\hat{t}$  satisfies the equation*

$$(M_0 \hat{t})(\xi) = 2^{-} \hat{t}(\xi) + r(\xi), \tag{5.48}$$

*where  $r(\xi)$  is a trigonometric polynomial, and  $(M_0 r)(\xi) = 2^{-} r(\xi)$ . Furthermore, we have*

$$r(\xi) = \sum_{1-2M}^{2M-1} r_n e^{in\xi},$$

*where the vector  $\mathbf{r} = \{r_{1-2M}, \dots, r_{2M-1}\}$  is given by*

$$\mathbf{b} - (\lambda I - A)\tau = \mathbf{r}.$$

*Thus, if the system (5.28) has a solution, then  $\mathbf{r} = 0$ , and in place of (5.48) we have*

$$(M_0 \hat{t})(\xi) = 2^{-} \hat{t}(\xi).$$

**Proof:** Let us define the trigonometric series

Then  $\hat{t}(\xi) = \sigma(\xi) + \tau(\xi)$ . We also define the trigonometric polynomial

$$b(\xi) = \sum_{1-2M}^{2M-1} b_n e^{in\xi},$$

here  $\mathbf{b} = \{b_{1-2M},$



# Bibliography

- [1] C. Anderson. A method of local corrections for computing the velocity field due to a distribution of vortex blobs. *Journal of Computational Physics*, 62, 1986.
- [2] G. Beylkin. On the representation

- [12] P. Ewald. Die berechnung optischer und elektrostatischer gitterpotentiale.  
*Annalen der Physik*, 64:

# Appendix A

## Solution of the System

$$\lambda x = Ax + b$$

In this appendix we consider solution of a linear system

$$\lambda x = Ax + b, \tag{A.1}$$

here  $A$  is a square, diagonalizable matrix, but is otherwise arbitrary. We assume that  $\lambda$  is an eigenvalue of  $A$  (otherwise there is no difficulty). When  $A$  is symmetric, the situation is well understood.

In the symmetric case, invariant subspaces belonging to distinct eigenvalues are orthogonal. If a symmetric matrix  $A$  has  $m$  distinct eigenvalues  $\lambda_1, \dots, \lambda_m$ , here  $m \leq n$ , and if  $P_i$  is the projector onto the invariant subspace belonging to  $\lambda_i$ , then we have the operator identity

$$I = P_1 + \dots + P_m,$$

called a partition of unity. Moreover, the system

$$\lambda_i x = Ax + b \tag{A.2}$$

has a solution if and only if  $P_i b = 0$ , and the solution is unique up to addition of an eigenvector of  $A$  belonging to  $\lambda_i$ .

It will be shown below that, even if  $A$  is not symmetric, a sequence of matrices  $D_i$  can be constructed that satisfies

$$I = D_1 + \dots + D_m,$$

the system (A.2) has a solution if and only if  $D_i b = 0$ , and the solution is unique up to addition of an eigenvector of  $A$  belonging to  $\lambda_i$ .

The matrices  $D_i$  imitate the projection matrices  $P_i$  in that they are idempotent ( $D_i^2 = D_i$ ), and satisfy  $D_i x = x \Leftrightarrow x = P_i x$ . However, they are not symmetric unless  $A$  is symmetric, in which case  $D_i = P_i$ .

In this appendix, we prove the following proposition.

**Proposition A.0.5** *Let  $A$  be a diagonalizable  $(n \times n)$  matrix. Let  $\lambda_1, \dots, \lambda$*

No set

$$D = R(L^T R)^{-1} L^T, \quad (\text{A.10})$$

here the linear independence of the columns of  $R$

N



since by Lemma(A.0.3)  $D_i v_j = 0$  if  $j \neq i$  and  $D_i v_i = v_i$ . It follows that (A.14) may be written as

$$x = D_1 x + \cdots + D_n x,$$

which implies the identity (A.5).

We now investigate the solution of (A.6). First note that Lemma(A.0.4) implies the existence of the inverse in (A.7). Write

$$r = b - (\lambda_i I - A)x. \tag{A.15}$$

Now,  $x$  is a solution to (A.6) if and only if  $r = 0$  in (A.15). Substituting the expression (A.7) for  $x$ , equation (A.15) becomes

$$\begin{aligned} r &= b - (\lambda_i I - A)x \\ &= b - (\lambda_i I - A)S_i(\lambda_i I - S_i^T A S_i)^{-1} S_i^T b \end{aligned}$$



# Appendix B

## Explicit Expression for $B_{m,n}(x)$

In this appendix we derive explicit expressions for the functions

$$B_{m,n}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ix\xi} \hat{\beta}^{(m)}(\xi - n\pi) \hat{\beta}^{(m)}(\xi + n\pi) d\xi. \quad (\text{B.1})$$

These are (Fourier transforms of) the functions  $\hat{\Phi}_n(\xi)$  introduced in Section 2.3.3, equation (2.67), in connection with the trigonometric expansion of a kernel. See also equation (3.23). Equation (B.1) corresponds to  $\Phi_n$  when the basis function is the central B-spline  $\beta^{(m)}(x)$ .

It will be more convenient for the derivation to use the B-spline  $N_m(x)$ , in place of  $\beta^{(m)}(x)$ . This notation is used by some authors (e.g. [5]) to denote the spline which is piecewise polynomial of degree  $(m-1)$ , and is supported on the interval  $[0, m]$ . The relationship between  $N_m(x)$  and  $\beta^{(m)}(x)$  is

$$\beta^{(m-1)}(x) = N_m(x + m/2).$$

It follows from this relationship that

$$\hat{N}_m(\xi - n\pi) \overline{\hat{N}_m(\xi + n\pi)} = \hat{\beta}^{(m-1)}(\xi - n\pi) \overline{\hat{\beta}^{(m-1)}(\xi + n\pi)}.$$

Thus, it is sufficient to prove the following proposition.

**Proposition B.0.6** *For  $m \geq 1$ , let  $N_m(x)$  denote the spline function which is piecewise polynomial of degree  $(m-1)$ , and which vanishes outside the interval  $[0, m]$ . Define*

$$B_{m-1,n}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ix\xi} \hat{N}_m(\xi - n\pi) \overline{\hat{N}_m(\xi + n\pi)} d\xi. \quad (\text{B.2})$$

Then, for  $n \geq 1$ , we have

$$B_{m-1,n}(x) = \sum_{k=0}^{m-1} \frac{(-i)^{m-k} a_{m,k}}{(2n\pi)^{m+k}} \left[ e^{in\pi x} + (-1)^{m-k} e^{-in\pi x} \right] \left( \frac{d}{dx} \right)^{m+k} N_{2m}(x + m), \quad (\text{B.3})$$

where

$$a_{m,k} = \frac{(m-1+k)!}{(m-1)!k!}. \quad (\text{B.4})$$

Note that the spline  $N_{2m}(x+m)$  is equal to the central B-spline of degree  $(2m-1)$ .

**Example:** Take  $m=4$ . The spline  $N_4(x+2)$  is equal to the central B-spline  $\beta^{(3)}(x)$ . When  $n=0$ , it is obvious that

$$B_{4,0}(x) = N_8(x+4) = \beta^{(7)}(x),$$

which is the autocorrelation of  $N_4(x)$ . If  $n \geq 1$ , then using the formula (B.3), we have  $B_{4,n}(x) =$

$$\left\{ \frac{\cos(n\pi x)}{8(n\pi)^4} \frac{d^4}{dx^4} - \frac{\sin(n\pi x)}{4(n\pi)^5} \frac{d^5}{dx^5} - \frac{5 \cos(n\pi x)}{16(n\pi)^6} \frac{d^6}{dx^6} + \frac{5 \sin(n\pi x)}{16(n\pi)^7} \frac{d^7}{dx^7} \right\} \beta^{(7)}(x).$$

Explicit expressions for the various derivatives of the central B-spline of degree seven are listed in the following table. We only consider  $x \geq 0$  since the central B-splines are even functions. Note also that the last column is piecewise constant, thus the seventh derivative does not exist at integer points, but since it is multiplied by the term  $\sin(n\pi x)$ , which is zero at integer points, this does not cause any discontinuity in the function

To prove the lemma, we use induction. First, consider

$$\begin{aligned}(e^{-i\xi} - 2 + e^{i\xi})e^{-ix\xi} &= e^{-i\xi(x+1)} - 2e^{-i\xi x} + e^{-i\xi(x-1)} \\ &= \Delta^2 e^{-i\xi(x+1)}.\end{aligned}$$

(In what follows, the algebra is somewhat tedious but entirely straightforward, and for the most part has been omitted.) Now, assume that (B.5) holds,

Similarly, expanding  $R_m(z)$  about  $z = -1$ , we have

$$\begin{aligned} R_m(z) &= \frac{f(z)}{(z+1)^m} \\ &= \frac{1}{(z+1)^m} \sum_{k=0}^{\infty} \frac{f^{(k)}(-1)}{k!} z^k \\ &= (-1)^m \sum_{k=0}^{\infty} a_{m,k} (z+1)^{k-m}. \end{aligned}$$

The partial fraction decomposition is the sum of the singular parts of these two expansions, which consists of the first  $(m-1)$  terms of each expansion. Combining these two finite sums gives (B.6).  $\square$

In (B.8), we consider the “function”  $F_m(x)$  as a formal expression only, which will be useful later on. We do not claim that the integral converges for all positive integers  $m$ .

**Lemma B.0.8** *Define*

$$F_m(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-ix\xi}}{\xi^m} d\xi, \quad m \geq 1. \quad (\text{B.8})$$

*These functions are related to the B-splines through the equation*

$$\Delta^m F_m(x) = (-i)^m N_m(x), \quad \text{a.e.} \quad (\text{B.9})$$

**Proof:** We first note that for  $m = 1$ , the integral is well-known, and we have

$$F_1(x) = \frac{-i}{\pi} \int_0^{\infty} \frac{\sin(x\xi)}{\xi} d\xi = \frac{-i}{2}$$

With this in hand, assume that (B.9) holds for index  $m - 1$ , and use (B.11) to compute

$$\begin{aligned}\Delta^m F_m(x) &= \Delta^m \frac{-ix}{m-1} F_{m-1}(x) \\ &= \frac{-i}{m-1} \sum_{n=0}^m \binom{m}{n} (\Delta^n x) \Delta^{m-n} F_{m-1}(x-n) \\ &= \frac{-i}{m-1} \left\{ \binom{m}{0} x \Delta^m F_{m-1}(x) + \binom{m}{1} \Delta^{m-1} F_{m-1}(x-1) \right\}.\end{aligned}$$

Here we have used the product formula for the back and difference operator, as well as the fact that  $\Delta^n x = 0$ , for  $n \geq 2$ . Now we have

$$\begin{aligned}\Delta^m F_m(x) &= \frac{-i}{m-1} \left\{ x \Delta^m F_{m-1}(x) + m \Delta^{m-1} F_{m-1}(x-1) \right\} \\ &= \frac{-ix}{m-1} \left[ \Delta^{m-1} F_{m-1}(x) - \Delta^{m-1} F_{m-1}(x-1) \right] \\ &\quad - \frac{im}{m-1} \Delta^{m-1} F_{m-1}(x-1) \\ &= \frac{-i}{m-1} \left\{ x \Delta^{m-1} F_{m-1}(x) + (m-x) \Delta^{m-1} F_{m-1}(x-1) \right\} \\ &= (-i)^m \left\{ \frac{x}{m-1} N_{m-1}(x) + \frac{m-x}{m-1} N_{m-1}(x-1) \right\} \\ &= (-i)^m N_m(x),\end{aligned}$$

here we have used (B.12) and our induction hypothesis.  $\square$

**Proof of Proposition:** Making the change of variable  $\xi \leftarrow \xi + n\pi$ , and using the formula

$$\hat{N}_m(\xi) = \left( \hat{N}_1(\xi) \right)^m = \left( \frac{e^{i\xi} - 1}{i\xi} \right)^m,$$

we can rewrite (B.2) as

$$\begin{aligned}e^{in\pi x} B_{m-1,n}(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ix\xi} \left( \frac{e^{i\xi} - 1}{i\xi} \right)^m \left( \frac{e^{-i\xi} - 1}{-i(\xi + 2n\pi)} \right)^m d\xi \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ix\xi} \frac{(e^{-i\xi} - 2 + e^{i\xi})^m}{[-\xi(\xi + 2n\pi)]^m} d\xi.\end{aligned}$$

Using Lemma(B.0.6), this equality can be written as

$$\begin{aligned}e^{in\pi x} B_{m-1,n}(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\Delta^{2m} e^{-i\xi(x+m)}}{[-\xi(\xi + 2n\pi)]^m} d\xi \\ &= \Delta^{2m} G_{m,n}(x+m),\end{aligned}$$

here we have put

$$G_{m,n}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-ix\xi}}{[-\xi(\xi + 2n\pi)]^m} d\xi.$$

Now, using Lemma(B.0.7), we can express the denominator of the integrand in the form

$$\begin{aligned} \frac{1}{[-\xi(\xi + 2n\pi)]^m} &= \frac{(-1)^m}{(2n\pi)^m} R_m \left( \frac{\xi}{2n\pi} \right) \\ &= \sum_{k=0}^{m-1} \frac{a_{m,k}}{(2n\pi)^{m+k}} \left\{ \frac{1}{(\xi + 2n\pi)^{m-k}} + \frac{(-1)^{m-k}}{\xi^{m-k}} \right\}. \end{aligned}$$

Using this equality, we can write

$$G_{m,n}(x) = \sum_{k=0}^{m-1} \frac{a_{m,k}}{(2n\pi)^{m+k}} [e^{2\pi i n x} + (-1)^{m-k}] \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-ix\xi}}{\xi^{m-k}} d\xi.$$

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