Chapter 1

Multiwavelet (MW) Basis

As stated on the previous chapter, the main goal of computational chemistry is to approximate systems in order to calculate their energy through the Schrödinger Equation (SE). These systems are completelly described by wave functions [4]. This means that to approximate a solution to the system is to approximate its wave function.

In order to construct a solution (wave function) to the SE of a given system one uses sets of orthogonal functions with differing properties. These sets of functions construct a basis for the space on which the wave functions are projected into. These sets are thus called basis sets [5] and they are essential to solving many body systems. In this text we will be focusing in the MW basis from Multi-Resolution Analysis (MRA) methods.

1.1 MRA

1.1.1 Definition

Consider that we have a function $\varphi \in L^2(\mathbb{R})$ where its tanslations and dilations are described as [9]

$$\varphi_k^j(x) = 2^{\frac{j}{2}}\varphi(2^j x - k),\ j,k \in \mathbb{Z} \tag{1.1}$$

. Where j is the scale of the function and k is the translation of the function [8] A space V_n is spanned by translations of φ_{nk}.This space forms a hierarchical chain of Linear subspaces [2]:

$$V_0 \subset V_1 \subset ... \subset V_j \subset ... \subset L^2(\mathbb{R}) \tag{1.2}$$

Where V_0 is spanned only by $\varphi_{0,0}(x) = \varphi(x)$ [8]. The function $\varphi(x)$ satisfies the two-scale difference relations [2, 9, 8]:

$$\begin{aligned} \varphi(x) &= \varphi(2x) + \varphi(2x-1) \\ \varphi_k^j(x) &= \varphi_{2k}^{j+1}(2^{j+1}x - 2k) + \varphi_{2k+1}^{j+1}(2^{j+1}x - 2k - 1) \end{aligned} \tag{1.3}$$

If relation 1.2 and the following refinement equation holds for $\varphi_{j,k}(x)$ one can call the subspaces V_n or the functions $\varphi_{j,k}(x)$ build a MRA of $L_2(\mathbb{R})$.

$$\varphi_k^j(x) = \sum_{k\in\mathbb{Z}} h_k^{j+1}\varphi_k^{j+1}(x) \tag{1.4}$$

Where h is a coefficient characteristic to the transformation between scales.

1.1.2 Wavelet MRA

Following from now we will work with the Haar wavelet basis for simplicity [2]. Lets define the Haar function [9] as

$$\varphi_0^0 = \varphi(x) = \begin{cases} 1 & \text{for } x \in [0,1) \\ 0 & \text{elsewhere} \end{cases} \tag{1.5}$$

Lets now define a second set of subspaces W_n. These are the orthogonal complements of V_n [1], also called difference subspaces, defined as [2, 8, 1].

$$W_n \oplus V_n = V_{n+1} \tag{1.6}$$

The subspaces W_n are then spanned by a set of functions defined by the translations and dilations of $\psi(x)$:

$$\psi_k^j(x) = 2^{\frac{j}{2}} \psi(2^j x - k), \ \ j, k \in \mathbb{Z} \tag{1.7}$$

Where $\psi(x)$ is called the Haar wavelet [9] and is defined as:

$$\psi_0^0 = \psi(x) = \begin{cases} 1 & \text{for } x \in [0, \frac{1}{2}) \\ -1 & \text{for } x \in [\frac{1}{2}, 1) \\ 0 & \text{elsewhere} \end{cases} \tag{1.8}$$

And φ is related to ψ by the following two-scale difference relation [2, 9, 8]:

$$\begin{aligned} \psi(x) &= \varphi(2x) - \varphi(2x-1) \\ \psi_k^j(x) &= \psi_{2k}^{j+1}(2^{j+1}x - 2k) + \psi_{2k+1}^{j+1}(2^{j+1}x - 2k - 1) \end{aligned} \tag{1.9}$$

The functions φ_k^j and ψ_k^j are orthonormal and dense [2, 8, 7] in $L^2(\mathbb{R})$.

The Definition on Equation 1.6 can be applied recursivelly in order to get any space V_n as long as one knows the first subspace V_0 and one has a method for constructing the subspace W_m from V_0 and W_{m-1}.

$$V_0 \oplus W_0 \oplus W_1 \oplus ... \oplus W_{n-1} = V_n \tag{1.10}$$

Projecting a function $f(x)$ unto this basis would be then a weighted linear combination of the Haar functions, but taking into account the definition on Equation 1.10 one arrives at [8].

$$f(x) \approx \sum_k^{2^j-1} \sum_j^N s_k^j \varphi_k^j = s_0^0 \varphi_0^0 + \sum_k^{2^j-1} \sum_j^{N-1} d_k^j \psi_k^j \tag{1.11}$$

where d are the difference coefficients and s are the scaled averages of dyadilic intervals of the function $f(x)$

The scaling coefficients s_k^j are computed by the projection $\langle \varphi_k^j(x) | f(x) \rangle$. Likewise the difference coefficients $d_k^j(x)$ are computed by the projection

$\langle \psi_k^j(x) | f(x) \rangle$. Because of the way the Haar function is defined, we can define of the scaling coefficients as scaled averages of $f(x)$ at intervals 2^{-j} [8, 2]

$$s_k^j = \int_{\mathbb{R}} \varphi_k^j(x) f(x) \mathrm{d}x = \int_{2^{-j}k}^{2^{-j}(k+1)} f(x) \mathrm{d}x \tag{1.12}$$

We can then obtain the difference coefficients by using Equations 1.12, 1.7 and 1.9:

$$\begin{aligned}
d_k^{j-1} &= \int_{\mathbb{R}} \psi_k^{j-1}(x) \mathrm{d}x \\
d_k^{j-1} &= 2^{\frac{j-1}{2}} \int_{\mathbb{R}} \psi(2^{j-1}x - k) f(x) \mathrm{d}x \\
d_k^{j-1} &= 2^{\frac{j-1}{2}} \left(\int_{\mathbb{R}} \varphi(2^j x - 2k) f(x) \mathrm{d}x - \int_{\mathbb{R}} \varphi(2^j x - 2k - 1) f(x) \mathrm{d}x \right) \\
d_k^{j-1} &= 2^{\frac{j-1}{2}} \left(\int_{2^{-j}2k}^{2^{-j}(2k+1)} f(x) \mathrm{d}x - \int_{2^{-j}(2k+1)}^{2^{-j}(2k+2)} f(x) \mathrm{d}x \right) \\
d_k^{j-1} &= \frac{1}{\sqrt{2}} \left(s_{2k}^j - s_{2k+1}^j \right)
\end{aligned} \tag{1.13}$$

The scaling coefficients can be obtained in the same manner:

$$\begin{aligned}
s_k^{j-1} &= \int_{\mathbb{R}} \varphi_k^{j-1}(x) \mathrm{d}x \\
s_k^{j-1} &= 2^{\frac{j-1}{2}} \int_{\mathbb{R}} \varphi(2^{j-1}x - k) f(x) \mathrm{d}x \\
s_k^{j-1} &= 2^{\frac{j-1}{2}} \left(\int_{\mathbb{R}} \varphi(2^j x - 2k) f(x) \mathrm{d}x + \int_{\mathbb{R}} \varphi(2^j x - 2k - 1) f(x) \mathrm{d}x \right) \\
s_k^{j-1} &= 2^{\frac{j-1}{2}} \left(\int_{2^{-j}2k}^{2^{-j}(2k+1)} f(x) \mathrm{d}x + \int_{2^{-j}(2k+1)}^{2^{-j}(2k+2)} f(x) \mathrm{d}x \right) \\
s_k^{j-1} &= \frac{1}{\sqrt{2}} \left(s_{2k}^j + s_{2k+1}^j \right)
\end{aligned} \tag{1.14}$$

The result of Equations 1.13 and 1.14 show us that we can represent the projection of coefficients unto a coarser scale as an orthogonal matrix [8, 2]:

$$\begin{pmatrix} d_k^j \\ s_k^j \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} s_{2k}^{j+1} \\ s_{2k+1}^{j+1} \end{pmatrix} \tag{1.15}$$

Projecting the coefficients into a more refined scale is just a transpose of the above matrix:

$$\begin{pmatrix} s_{2k}^{j+1} \\ s_{2k+1}^{j+1} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} d_k^j \\ s_k^j \end{pmatrix} \tag{1.16}$$

1.1.3 Projecting a gaussian function example

As an example, lets approximate the function $f(x) = \frac{10}{\sqrt{\pi}} e^{-100(x-0.5)^2}$ in $L^2(\mathbb{R})$ with Haar basis up to scale 5 using 1.11. Gives us the following figures.

1.2 MW MRA

1.2.1 Constructing the basis functions in one dimension

Following the same basics as in the Haar basis from the previous section we can define a hierarchical set of multiresolution spaces V_j^l where [6]:

$$\begin{aligned} V_j^l \stackrel{\text{def}}{=} \{f :& \text{ all polynomials of degree} \leqslant l \\ & \text{on } (2^{-j}k, 2^{-j}(k+1)) \text{ for } 0 \leqslant k < 2^n, \\ & f \text{ vanishes elsewhere}\} \end{aligned} \tag{1.17}$$

and

$$V_0^l \subset V_1^l \subset ... \subset V_j^l \subset ... \subset L^2(\mathbb{R}) \tag{1.18}$$

We again define subspaces W_j^l as the orthogonal complements of V_j^l [1] defined as:

$$V_j^l \oplus W_j^l = V_{j+1}^l \tag{1.19}$$

with orthogonal basis functions h_{lk}^j which are translations and dilations of functions h_l:

$$h_{ik}^j(x) = 2^{\frac{j}{2}} h_i(2^j x - k),\ i = 1, ..., l;\ k \in \mathbb{Z} \tag{1.20}$$

The functions $h_1, ..., h_l$ are piecewise polynomial, orthogonal to lower order polynomials and vanish outside $[0, 1]$ [1]

$$\int_0^1 h_i(x) x^m \mathrm{d}x = 0,\ m = 0, 1, ..., l-1 \tag{1.21}$$

Our aim is to find a set of functions f_i on the interval $[-1, 1]$ that can be used in the construction of $h_1, ..., h_l$ with the following restrictions [1, 2]:

1. functions f_i on the interval $(0, 1)$ are polynomials of degree $l - 1$.
2. functions f_i extend to the interval $(-1, 0)$ as even or odd functions dependendent to the parity $i + l - 1$.
3. functions $f_1, ..., f_l$ satisfy :
$$\int_{-1}^1 f_i(x) f_j(x) \mathrm{d}x \equiv \langle f_j | f_j \rangle = \delta_{ij},\ i, i = 1, ..., l.$$
4. functions f_j have vanishing moments,
$$\int_{-1}^1 f_j(x) x^i \mathrm{d}x = 0,\ i = 0, 1, ..., j + l - 2.$$

The functions $f_1^{(1)}, f_2^{(1)}, ..., f_l^{(1)}$ are defined by [1]:

$$f_j^1(x) = \begin{cases} x^{j-1} & \text{for } x \in (0, 1) \\ -x^{j-1} & \text{for } x \in (-1, 0) \\ 0 & \text{elsewhere.} \end{cases} \tag{1.22}$$

The $2l$ functions $1, x, ..., x^{l-1}$ and $f_1^{(1)}, f_2^{(1)}, ..., f_l^{(1)}$ are linearly independent, thus they span the space of polynomial functions of degree $< l$ on the intervals $(0, 1)$ and $(-1, 0)$ [1, 2]. We do the following process to find the functions f_i [1]:

1. Using the Gram-Schmidt process we orthogonalize $f_j^{(1)}$ with respect to $1, x, ..., x^{l-1}$ giving us the functions $f_j^{(2)}$ for $j = 1, ..., l$.

2. We try to find at least one $f_j^{(2)}$ which is not orthogonal to x^l and reorder the functions so that $\langle f_1^{(2)} | x^l \rangle \neq 0$. We now need to find an a_j for the equation $f_j^{(3)} = f_j^{(2)} - a_j \cdot f_0^{(2)}$ such that $\langle f_j^{(3)} | x^l \rangle = 0$ for $l = 2, ..., l$. We repeat this process orthogonalizing to $x^{k+1}, ..., x^{2k-2}$, each turn yielding $f_1^{(2)}, f_2^{(3)}, f_3^{(4)}, ..., f_k^{(k+1)}$ such that $\langle f_j^{(j+1)} | x^i \rangle = 0$ for $i \leqslant j + l - 2$.

3. Lastly we perform the Gram-Schmidt orthogonalization process on f_l^{l+1}, $f_{l-1}^{l}, f_{l-2}^{l-1}, ..., f_2^1$ in that order to get $f_l, f_{l-1}, ..., f_1$.

We now construct the functions h_l [1]:

$$h_i(x) = \sqrt{2} f_i(2x - 1),\ i = 1, ..., l \tag{1.23}$$

which they themselves build the functions in Equation 1.20 defining a basis for scaling subspace W_j^l.

From the definition of these subspaces we know that we need to define a basis for the subspace V_0^l which is the orthogonal complement of W_0^l in V_1^l [1]. The basis functions $u_i(x)$ of the subspace V_0^l can be defined using the following two-scale difference equations [3], which are analogous to the two-scale difference equations in 1.9.

$$h_i(x) = \sqrt{2} \sum_{j=0}^{l-1} \left(\bar{H}_{ij}^{(0)} h_j(2x) + \bar{H}_{ij}^{(1)} h_j(2x - 1) \right),\ i = 0, ..., l - 1 \tag{1.24}$$

$$u_i(x) = \sqrt{2} \sum_{j=0}^{l-1} \left(\bar{G}_{ij}^{(0)} h_j(2x) + \bar{G}_{ij}^{(1)} h_j(2x - 1) \right),\ i = 0, ..., l - 1 \tag{1.25}$$

Where $\bar{H}$ and $\bar{G}$ are quadrature mirror filter matrices [3] which have the following properties:

$$\bar{H}^{(0)} \bar{H}^{(0)T} + \bar{H}^{(1)} \bar{H}^{(1)T} = \bar{I} \tag{1.26}$$

$$\bar{G}^{(0)} \bar{G}^{(0)T} + \bar{G}^{(1)} \bar{G}^{(1)T} = \bar{I} \tag{1.27}$$

$$\bar{H}^{(0)} \bar{G}^{(0)T} + \bar{H}^{(1)} \bar{G}^{(1)T} = \bar{0} \tag{1.28}$$

Which can be summarized in the orthogonal block matrix $\bar{U}$ [3]

$$\bar{U} = \begin{pmatrix} \bar{H}^{(0)} & \bar{H}^{(1)} \\ \bar{G}^{(0)} & \bar{G}^{(1)} \end{pmatrix} \tag{1.29}$$

Which lets us put the two two-scale difference equations in the following way [8]

$$\begin{pmatrix} \vec{h}(x) \\ \vec{u}(x) \end{pmatrix} = \sqrt{2} \begin{pmatrix} \bar{H}^{(0)} & \bar{H}^{(1)} \\ \bar{G}^{(0)} & \bar{G}^{(1)} \end{pmatrix} \begin{pmatrix} \vec{h}(2x) \\ \vec{h}(2x - 1) \end{pmatrix} \tag{1.30}$$

and subsequently

$$\begin{pmatrix} \vec{h}(2x) \\ \vec{h}(2x - 1) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \bar{H}^{(0)} & \bar{G}^{(0)} \\ \bar{H}^{(1)} & \bar{G}^{(1)} \end{pmatrix} \begin{pmatrix} \vec{h}(x) \\ \vec{u}(x) \end{pmatrix} \tag{1.31}$$

1.2.2 Choices of Scaling functions

Now that we have stated how to build the scaling and wavelet basis functions we need to make a choice of functions f to build said basis. Here we will breifly show two examples of polunomial functions used to create the basis. These two are the Legendre polynomials and the Lagrange interpolating polynomials [2, 3]

Legendre basis The Legendre scaling function is defined as follows

$$\phi_j(x) \begin{cases} \sqrt{2j+1}P_j(2x-1),\ x & \in [0,1) \\ 0,\ x & \notin (0,1) \end{cases} \tag{1.32}$$

Where P_j are the Legendre polynomials of order j defined in $[-1,1]$ [2] Following are some examples of the polynomials together with figures of the first few terms of the functions. These functions have the advantage of being simple to compute, since each incremental polynomial order only adds a single term to the function.

Lagrange interpolating basis

$$\varphi = \frac{1}{\sqrt{w_i}} l_i(x),\ i = 0, ..., M-1 \tag{1.33}$$

$$l_i(x) = \prod_{k=0,k\neq i}^{M-1} \frac{x - x_k}{x_i - x_k} \tag{1.34}$$

$$w_i = \frac{1}{MP'_M(2x_i - 1)P_{M-1}(2x_i - 1)} \tag{1.35}$$

Where M is the scale of the subspace, the P functions are the Legendre polynomials and $x_0, ..., x_{M-1}$ are the roots of $P_M(2x-1)$ [2]. These scaling functions have the characteristic of $l_i(x_j) = \delta_{ij}$ simplifying integrals and thus projections of the basis.

Going from one dimension to d dimensions is to use a tensor product method as shown in [6].

1.3 Operators

1.3.1 Nonstandard (NS) form Representation of Operators

Lets us define two projection operators P_n^k and Q_n^k and their relation as:

$$P_n^k :\ L^2([0,1]) \to V_n^k \tag{1.36}$$

$$Q_n^k :\ L^2([0,1]) \to W_n^k \tag{1.37}$$

$$Q_n^k = P_{n+1}^k - P_n^k \tag{1.38}$$

A function f would then be projected into a scale n by $f_n^k = P_n^k f$. Its projection unto a more refined scale would then be $f_{n+1}^k = f_n^k + df_n^l$ where $df_n^k = Q_n^k f$ [6].

We expand a linear operator $T: L^2([0,1]) \to L^2([0,1])$ as

$$
\begin{aligned}
T &= P_0^k T P_0^k + \sum_{n=0}^{\infty} \left(P_{n+1}^k T P_{n+1}^k - P_n^k T P_n^k \right) \\
&= P_0^k T P_0^k + \sum_{n=0}^{\infty} \left((P_n^k + Q_n^k) T (P_n^k + Q_n^k) - P_n^k T P_n^k \right) \\
&= P_0^k T P_0^k + \sum_{n=0}^{\infty} \left(P_n^k T Q_n^k + Q_n^k T P_n^k + Q_n^k T Q_n^k \right)
\end{aligned}
\tag{1.39}
$$

We represent the operator T as

$$A_n^k \stackrel{\text{def}}{=} Q_n^k T Q_n^k : W_n^k \to W_n^k \tag{1.40}$$

$$B_n^k \stackrel{\text{def}}{=} Q_n^k T P_n^k : V_n^k \to W_n^k \tag{1.41}$$

$$C_n^k \stackrel{\text{def}}{=} P_n^k T Q_n^k : W_n^k \to V_n^k \tag{1.42}$$

$$T_n^k \stackrel{\text{def}}{=} P_0^k T P_0^k : V_n^k \to V_n^k \tag{1.43}$$

so we can write the NS form of the operator T as [6, 3]

$$T = T_0^k + \sum_{n=0}^{\infty} \left(A_n^k + B_n^k + C_n^k \right) \tag{1.44}$$

We can then apply T on f and get, by using the definitions above, the following result:

$$
\begin{aligned}
Tf = g &= \hat{g}_0^k + \sum_{n=0}^{\infty} \left(\tilde{g}_n^k + d\tilde{g}_n^k \right) \\
&= T_0^k f_0^k + \sum_{n=0}^{\infty} \left((A_n^k + C_n^k) df_n^k + B_n^k f_n^k \right) \\
\hat{g}_n^k &\stackrel{\text{def}}{=} T_n^k f = T_n^k f_n^k \\
\tilde{g}_n^k &\stackrel{\text{def}}{=} C_n^k f = C_n^k f_n^k \\
d\tilde{g}_n^k &\stackrel{\text{def}}{=} \left(A_n^k + B_n^k \right) f = A_n^k f_n^k + B_n^k f_n^k
\end{aligned}
\tag{1.45}
$$

In practice we truncate this to the fines scale $N+1$ where the following is assumed to be true [6]:

$$\hat{g}_{N+1}^k \simeq g_{N+1}^k \stackrel{\text{def}}{=} (Tf)_{N+1}^k \tag{1.46}$$

Assuming that the operator is separable as a tensor product, one can define it in d dimensions in much the same way as with the scaling functions with tensor products across the dimensions d. In [6] the kernel of the tensor operator is described as a linear combination of one dimensional kernels, thus simplifying the problem from k^d vector elements to just k vector elements.

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