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 [3]. 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 [4] 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 [8]

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

. Where j is the scale of the function and k is the translation of the function [7] 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 $\varphi_{0,0}(x) = \varphi(x)$ [7]. The function $\varphi(x)$ satisfies the two-scale difference relations [2, 8, 7]:

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

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 [8] 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, 7, 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 [8] 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, 8, 7]:

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

The functions φ_k^j and ψ_k^j are orthonormal and dense [2, 7, 6] 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 [7].

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

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

$\langle \psi^j_k(x) | f(x) \rangle$. 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} [7, 2]

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

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

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

The scaling coefficients can be obtained in the same manner:

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

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 [7, 2]:

$$\begin{pmatrix} d^j_k \\ s^j_k \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} s^{j+1}_{2k} \\ s^{j+1}_{2k+1} \end{pmatrix} \tag{1.15}$$

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

$$\begin{pmatrix} s^{j+1}_{2k} \\ s^{j+1}_{2k+1} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} d^j_k \\ s^j_k \end{pmatrix} \tag{1.16}$$

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 Defining the basis functions

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 [5]:

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

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 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

1.2.2 Interpolating basis

1.2.3 Operators

1.2.4 Functions

1.3 Solving systems

1.3.1 Integral equations

1.3.2 Differential equations

1.4 Software

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