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 [2]. 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 [3] 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 [6]

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

. Where j is the scale of the function and k is the translation of the function [5] A space V_n is spanned by translations of φ_{nk}.This space forms a hierarchical chain of Linear subspaces [1]:

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

Where V_0 is spanned only by $\varphi_{0,0}(x) = \varphi(x)$ [5]. The function $\varphi(x)$ satisfies the two-scale difference relations [1, 6, 5]:

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

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 [1]. Lets define the Haar function [6] 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 difference subspaces defined as [1, 5]

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

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

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

Where $\psi(x)$ is called the Haar wavelet [6] 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 [1, 6, 5]:

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

The functions φ_k^j and ψ_k^j are orthonormal and dense [1, 5, 4] in $\mathbb{L}^2(\mathbb{R})$.

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 [5].

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

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} [5, 1]

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

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 [5, 1]:

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

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

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

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

1.2 The MW Basis

1.2.1 Constructing The Basis

Polynomials

Scale

World size

Precision threshold

1.2.2 Operators

1.2.3 Functions

1.3 Solving systems

1.3.1 Integral equations

1.3.2 Differential equations

1.4 Software

Bibliography

[1] Gregory Beylkin. Lecture notes on mra/madness.

[2] Claude Cohen-Tannoudji, Bernard Diu, and Franck Laloë. *Quantum Mechanincs*, volume one. Wiley-Interscience, 1973.

[3] Cristopher J. Cramer. *Essentials of to Computational Chemistry: Theories and models.* Wiley, 2 edition, 2004.

[4] Stig Rune Jensen. *Real-space all-electron Density Functional Theory with Multiwavelets.* PhD thesis, UiT, The arctic university of norway, 2 2014.

[5] Rune Sørland Monstad. Solvent effects with multiwavelets. Master's thesis, UiT, The arctic university of norway, 11 2017.

[6] R. Schneider and F. Krüger. Introduction to multiresolution analysis (mra). TUB - Technichal University of Berlin, Jan. 22 2007.