Journal

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Week 1 (09/08/08-09/12/08)

This is the first week of the new fall quarter. And the subject I need to work on is also totally new on Fast Adaptive Algorithms in the Non-standard Form for Multidimensional Problems. This algorithm present a fast, adaptive multiresolution algorithm for applying integral operators with a wide class of radially symmetric kernels in dimensions one, two and three. Related papers provide the algorithm for the Poisson and *Shrödinger* equations in dimension three. The same algorithm may be used for all operators with radially symmetric kernels approximated as a weighted sum of Gaussians, making it applicable across multiple fields by reusing a single implementation.

Week 2 (09/15/08-09/19/08)

This week, I am trying to understand the basic idea of the multiresolution representations of kernels and use multiwavelet bases that a method for discretizing integral equations, as is the case in quantum chemistry. I will briefly describe the multiresolution analysis, especially the adaptive representation of functions during the meeting next week.

Next week, I will go further to see the combination of the separated and multiresolution representations of kernels.

Week 3 (09/22/08-09/26/08)

This week, I continued to read the first paper on the algorithms for multidimensional problems. Dr. Martin explained the algorithm of modified ns-form in 1D to me. This helped me to have a better understanding of the algorithm 2 of this paper. But, I found my understanding of algorithm 2 had some differences with Dr. Martin's. So, I need to discuss this with him next week.

Next week, Dr. Martin will give a speech based on the second paper. I plan to start reading the second paper after this speech.

Week 4 (09/29/08-10/03/08)

After the speech given by Dr. Martin, I started to read the paper the speech based on, which is apply the unconstrained sum of slater determinants to approximate a wave function. This paper used the fast adaptive algorithms mentioned in previous paper to handle the operators, applies the sum of slater determinants to approximate the wavefunction and the separated representation is also applied in this paper to meet the requirement of accuracy and efficiency for high dimensional problems.

Week 5 (10/06/08-10/10/08)

This week, I tried to understand the basic algorithm of the 'slater determinant' paper. The basic idea of this paper is very clear, however, there are lots of details in this paper. The reason is that we need to handle the operators and the wavefunction at the same time. First, for the operators, we can apply the adaptive representations, and for the wavefunctions, we can apply the slater determinant, especially the separable representation of slater determinant to approximate the wavefunctions.

Next week, I will go into the details of the algorithm mentioned in this paper and try to understand the proofs.

Week 6 (10/13/08-10/17/08)

This week, I am still reading the 'slater determinant' paper.

In this paper, we hope to find the coefficients $\{c_i\}$ to minimize

$$||f - \sum_i c_i g_i||^2 =< f - \sum_i c_i f_i, f - \sum_i c_i f_i >$$

construct the normal equations

$$Ax = b$$

with

$$A(k,i) =< g_k, g_i > \quad and \quad b(k) =< g_k, f >$$

solve them, and set $c_i = x(i)$.

The presentation of A and b are:

$$A(l,l')(\gamma,\gamma') = \tilde{s_l}\tilde{s_{l'}} < \delta(\gamma - \gamma_1)\prod_{i=2}^{N}\tilde{\phi}_i^l(\gamma_i), \delta(\gamma' - \gamma_1)\prod_{i=2}^{N}\tilde{\phi}_i^{l'}(\gamma_i) >$$

$$b(l)(\gamma) = \tilde{s_l}\sum_m^r s_m < \delta(\gamma - \gamma_1)\prod_{i=2}^{N}\tilde{\phi}_i^l(\gamma_i), -G_\mu[V + W]\prod_{i=1}^{N}\tilde{\phi}_i^m(\gamma_i) >$$

Hence, the most important job is to construct A and b, which includes:

1. Antisymmetric inner product with the electron-electron potential W
2. Antisymmetric inner product with T and/or V present
3. Antisymmetric inner product with $\delta(\gamma - \gamma_1)$ and $(T \textit{ and/or } V)$ present
4. Antisymmetric inner product with $\delta(\gamma - \gamma_1)$ and W present

Week 7 (10/20/08-10/24/08)

This week, I basically finished reading the 'Slater determinants' paper. I found the method used in handling the Green's function is similar to the way I learnt in the previous 'Multiresolution' paper. Actually, the 'Multiresolution' paper can solve for the operator in the form of $(-\Delta + \mu^2 I)^{-\alpha}$, when $\mu \geq 0$ and $0 < \alpha < 3/2$. The Green's function

$$G_\mu = (T - \mu I)^{-1} \qquad\qquad T = -\frac{1}{2}\sum_{i=1}^{N} \Delta_i$$

is a special case of the operator mentioned above. Therefore, we can directly apply the multiresolution method in approximating the wavefunction for the multiparticle Schr*ö*dinger equation.

Next week, I will begin to prepare for the final presentation and start reading the new paper based on the previous two papers.

Week 8 (10/27/08-10/31/08)

This week, I was preparing for the final presentation. I went through all the papers I read this quarter and found that they were easier for me to understand than a few weeks ago. I had a better understanding of Prof. Martin's research and the problems we hoped to solve. But, in the process of preparing for the final presentation, I found I still had some questions about the previous papers. I might need to reconsider these questions one by one.

This week, I also started to read the new paper based on the previous two papers. The first part of the paper is not difficult to understand. It is a review of the previous papers. And then, the paper focus on the errors involved in each step of approximation. I will look into the details of the error analysis next week.

Week 9 (11/3/08-11/7/08)

This week, I gave the final presentation. This presentation encouraged me to go back to the beginning of this quarter and went over the papers I read a few weeks before, even the very first 'Multivariate Regression' paper to review the separate representation

I thought the final presentation is not that good as I expected. I should explain some things more clear than I did. And after the presentation, I decided to go over the codes of the related methods which can help me to understand the actual procedures we applied to realize the algorithms.

Week 10 (11/10/08-11/14/08)

After the final presentation, I continued to read the new paper written by Prof. Martin. In this paper, it mentioned that in order to accomplish the algorithm we discussed on week 6, the numerical method for representing and operating on the functions ϕ_i^l needs to perform

$$\phi \mapsto \phi\theta \mapsto |L| \int V(r)\phi(r)\theta(r)dr \tag{1}$$

$$\phi \mapsto \phi\theta \mapsto W_p[\phi\theta] \mapsto |L| \int \phi(r)\theta(r)W_p[\phi\theta]dr \tag{2}$$

$$\phi \mapsto V_*[\phi] \mapsto |E|FV_*[\phi] \tag{3}$$

$$\phi \mapsto \phi\widetilde{\theta} \mapsto W_p[\phi\widetilde{\theta}] \mapsto \phi W_p[\phi\widetilde{\theta}] \mapsto |E|F\phi W_p[\phi\widetilde{\theta}] \tag{4}$$

The sequences (1) and (2) produce numbers, so our requirement for the numerical method is that it compute these numbers to any requested accuracy. The sequences (3) and (4) are used to produce undated functions ϕ, so our requirement is a bit more subtle. What I did this week is to understand the requirements enforced on each step of approximations.

For the nuclear potential in an inner product, we look at the worst behavior at the origin, which is the core orbital. In order to assure the relative (or absolute) error ϵ, we have to make sure $\delta < \sqrt{\frac{3\epsilon}{2}}\frac{1}{z^2}$ to achieve absolute error or to make sure $\delta < \sqrt{\frac{3\epsilon}{2}}\frac{1}{z}$ to achieve relative error ϵ. And for the action on the function error, the constant α should fulfill $\alpha < \frac{\epsilon}{16Z^2}$.

For the inter-electron potential in an inner product, in order to achieve the relative error ϵ, we need $\delta < \sqrt{\frac{5\epsilon}{3}}\frac{1}{4z}$, $\nu\sqrt{D} < \frac{5\epsilon}{3.8\sqrt{2Z}}$ and $\eta < \frac{5Z\epsilon}{3.8}$. And for the action on the function error, we need $\alpha\sqrt{D} < \frac{\epsilon}{4\sqrt{Z^3}}$ to maintain absolute error ϵ.

This is not the end of the error analysis. To be continued after the final week.