An Optimised Sparse Grid Combination Technique for Eigenproblems

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We introduce the optimised sparse grid combination technique for the numerical solution of d-dimensional eigenproblems on sparse grids. We present numerical results for the stationary Schrödinger equation in the case of hydrogen.

1 Introduction

In this paper we consider the eigenvalue problem resulting from the Born-Oppenheimer approximation of the stationary Schrödinger equation for atoms. Following [1] we employ a finite element discretisation with piecewise d-linear test and trial functions which leads to a discrete eigenvalue problem. To partially cope with the curse of dimensionality of finite element discretisations the sparse grid combination technique is applied. For a d-dimensional problem, the sparse grid approach employs only $\mathcal{O}(h_n^{-1}(\log h_n^{-1})^{d-1})$ grid points in the discretisation, where h_n is the finest mesh size in one dimension.

The combination technique uses a certain sequence of anisotropic grids with a nodal discretisation. A linear combination of the corresponding partial solutions on each grid then gives a sparse grid representation. In general this is not the solution which one would achieve working directly in the sparse grid space using a hierarchical basis. But, under certain assumptions on the error expansion on the partial grids, the same convergence behaviour can be shown for the combination technique and the direct sparse grid approach [2]. On the other hand, empirical results in machine learning applications show divergence of the combination technique in certain situations [3]; here these assumptions do not hold. In [3] the behaviour of the sparse grid combination technique is investigated in more detail, in particular is the solution of the underlying problem viewed as a projection. One can show that the difference between the combination of the partial projections and the projection into the underlying sparse grid space can be large if the projections into the partial spaces do not commute.

Applying a so-called optimised combination technique, in short opticom, repairs the resulting instabilities of the combination technique [3]. The combination coefficients now not only depend on the grids involved, but on the function to be represented as well, resulting in a non-linear approximation approach.

Due to the singularities present, the solutions of the Schrödinger equation will not have the necessary error expansion from [2]. Since the opticom approach was introduced in a projection framework it cannot directly be applied to eigenvalue-problems. In this paper we will show how one can reformulate the projection setting for the optimised combination technique as a Galerkin-approach using the partial solutions as ansatz functions. This view is valid for eigenvalue problems as well.

2 Numerical Approach

We consider the stationary Schrödinger equation which gives the eigenvalue equation $Hu = Eu$, or in weak form $a(u,\psi) := \langle Hu,\psi\rangle = E\langle u,\psi\rangle \quad \forall\psi$. We use the Born-Oppenheimer approximation, and get for hydrogen the electronic Hamilton operator $-\Delta u(\underline{x}) - \frac{2}{|\underline{x}|}u(\underline{x})$ in atomic units. We restrict ourselves to a bounded domain $\Omega = [-a,a]^d$, which introduces some error, using Dirichlet boundary conditions.

The combination technique [2] considers all grids $\Omega_{\underline{l}} = \Omega_{l_1,\ldots,l_d}$ with indices $|\underline{l}|_1 := l_1 + \ldots + l_d = n + (d-1) - q, q = 0,..,d-1, l_t > 0$ and a finite element discretisation using piecewise d-linear test and trial functions of uniform mesh size $h_t = 2a \cdot 2^{-l_t}$ in the t-th direction. The partial solutions $f_{\underline{l}}$ from each grid are combined to get the solution f_n^c on the corresponding sparse grid using the formula

$$f_n^c = \sum_{q=0}^{d-1} (-1)^q \binom{d-1}{l} \sum_{|\underline{l}|_1 = n+(d-1)-q} f_{\underline{l}}. \tag{1}$$

The resulting function f_n^c lives in a so-called sparse grid space V_n^s of dimension $\mathcal{O}(h_n^{-1}(\log h_n^{-1})^{d-1})$. For more details on the combination technique for eigenvalue problems see [1].

In [3] the combination technique is studied as a projection with the scalar product $\langle\cdot,\cdot\rangle_a$ defined by the bilinear operator $a(\cdot,\cdot)$ in the Galerkin equations of the problem to be solved. That way the approximation of a sparse grid function by the combination of partial functions can be viewed as the minimisation problem $\min J(c_1,\ldots,c_k)$ with $J(c_1,\ldots,c_k) =$

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$\|P_{V_n^s}\hat{f} - \sum_{l=1}^{k} c_l P_l \hat{f}\|_a^2$, here $P_{V_n^s}\hat{f}$ denotes the projection of the continuous solution $\hat{f}$ into the sparse grid space and $P_l\hat{f}$ is the projection into a partial space (we use here a suitable numbering scheme). The projection into a discrete space is the solution of the discretised problem in the Galerkin formulation, i.e., $a(P_l\hat{f}, v) = R(v) \quad \forall v \in V_l$, where $R(\cdot)$ denotes the functional on the right hand side. The goal is now to approximate the sparse grid solution (whose direct computation is infeasible in some situations due to computational constraints) with a combination of partial solutions. It turns out that, using (1), the combination solution is exact, and therefore $J = 0$, only if the projections onto the partial grids Ω_l commute, which is not the case for partial differential equations [3].

But optimal combination coefficients can be computed if one minimises the equation with regard to the c_l. Simple expansion gives $J(c_1, \ldots, c_k) = \sum_{l,j=1}^{k} c_l c_j \langle P_l\hat{f}, P_j\hat{f}\rangle_a - 2\sum_{l=1}^{k} c_l \|P_l\hat{f}\|_a^2 + \|P_{V_n^s}\hat{f}\|_a^2$, and since the location of the minimum of J does not depend on $P_{V_n^s}f$, the best combination coefficients satisfy (after derivation with regard to c_l)

$$\begin{bmatrix} \langle P_1\hat{f}, P_1\hat{f}\rangle_a & \cdots & \langle P_1\hat{f}, P_k\hat{f}\rangle_a \\ \langle P_2\hat{f}, P_1\hat{f}\rangle_a & \cdots & \langle P_2\hat{f}, P_k\hat{f}\rangle_a \\ \vdots & \ddots & \vdots \\ \langle P_k\hat{f}, P_1\hat{f}\rangle_a & \cdots & \langle P_k\hat{f}, P_k\hat{f}\rangle_a \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_k \end{bmatrix} = \begin{bmatrix} \|P_1\hat{f}\|_a^2 \\ \|P_2\hat{f}\|_a^2 \\ \vdots \\ \|P_k\hat{f}\|_a^2 \end{bmatrix} = \begin{bmatrix} R(P_1\hat{f}) \\ R(P_2\hat{f}) \\ \vdots \\ R(P_k\hat{f}) \end{bmatrix}$$

We here observe that $\|P\hat{f}\|_a^2 = R(P\hat{f})$ holds for the solution $P\hat{f}$ of the Galerkin formulation. We therefore can interpret the optimised combination technique, i.e., the sum of projections into the partial spaces with the opticom coefficients, as a Galerkin formulation which uses the partial solution $P_l\hat{f}$ as ansatz functions. While the projection arguments do not hold for the eigenvalue problem, the Galerkin view does hold in this case as well.

3 Numerical Results

We now use the eigensolutions from the sequence of grids in (1) as basis functions for a new eigenvalue problem, which is a full but small matrix of size #grids × #grids. It consists of the mixed terms $a(P_l\hat{f}, P_k\hat{f})$ and $\langle P_l\hat{f}, P_k\hat{f}\rangle$. Note that in [1] the eigenvalues were computed using the formula $\sum_{l=1}^{k} c_l RQ(P_l\hat{f})$, where c_l is the combination coefficient from equation (1) and RQ denotes the Rayleigh quotient $RQ(f) = \frac{a(f,f)}{\langle f,f\rangle}$. This is only an approximation to the Rayleigh quotient of the combination technique $RQ(f_n^c)$ which includes the above mixed terms in its expansion over the partial solutions. Therefore there is little overhead for the opticom approach with regard to the correct form of the combination technique since only a small additional eigenvalue problem needs to be solved.

In Table 1 we present numerical results for the case of hydrogen, this problem is a three-dimensional one. We give the results from [1], use the correct Rayleigh quotient for the combination technique, and use the optimised combination technique. We observe significant gains with the opticom approach, the error is reduced by a factor of 14 compared with the published results from [1] and a factor of 5 against the combination technique with the correct Rayleigh quotient including the mixed terms $a(P_l\hat{f}, P_k\hat{f})$ and $\langle P_l\hat{f}, P_k\hat{f}\rangle$.

Table 1 Results for ground state of hydrogen from [1] (left) compared with the combination technique with the correct Rayleigh quotient (middle) and the optimised combination technique (right). Note that the exact value is -1.0.

	[1]			$RQ(f_n^c) = \frac{a(f_n^c, f_n^c)}{(f_n^c, f_n^c)}$			opticom		
n	λ_n	e_n	$\frac{e_{n-1}}{e_n}$	λ_n	e_n	$\frac{e_{n-1}}{e_n}$	λ_n	e_n	$\frac{e_{n-1}}{e_n}$
4	-0.75376	$2.462{\cdot}10^{-1}$	-	-0.75376	$2.462{\cdot}10^{-1}$		-0.75376	$2.462{\cdot}10^{-1}$	
5	-0.77119	$2.288{\cdot}10^{-1}$	1.08	-0.77151	$2.285{\cdot}10^{-1}$	1.07	-0.77151	$2.285{\cdot}10^{-1}$	1.07
6	-0.88938	$1.110{\cdot}10^{-1}$	2.07	-0.90223	$9.777{\cdot}10^{-2}$	2.33	-0.90387	$9.612{\cdot}10^{-2}$	2.37
7	-0.92932	$7.067{\cdot}10^{-2}$	1.57	-0.95163	$4.484{\cdot}10^{-2}$	2.02	-0.95507	$4.492{\cdot}10^{-2}$	2.13
8	-0.96595	$3.404{\cdot}10^{-2}$	2.08	-0.97848	$2.151{\cdot}10^{-2}$	2.24	-0.98022	$1.977{\cdot}10^{-2}$	2.27
9	-0.98378	$1.621{\cdot}10^{-2}$	2.10	-0.99259	$7.405{\cdot}10^{-3}$	2.90	-0.99364	$6.350{\cdot}10^{-3}$	3.11
10	-0.99321	$6.787{\cdot}10^{-3}$	2.39	-0.99729	$2.709{\cdot}10^{-3}$	2.73	-0.99812	$1.875{\cdot}10^{-3}$	3.38
11	-0.99741	$2.585{\cdot}10^{-3}$	2.63	-0.99919	$8.032{\cdot}10^{-4}$	3.37	-0.99954	$4.583{\cdot}10^{-4}$	4.09
12	-0.99879	$1.204{\cdot}10^{-3}$	2.15	-0.99953	$4.630{\cdot}10^{-4}$	1.73	-0.999914	$8.586{\cdot}10^{-5}$	5.34

References

[1] J. Garcke and M. Griebel, Journal of Computational Physics **165**(2), 694–716 (2000).
[2] M. Griebel, M. Schneider, and C. Zenger, A combination technique for the solution of sparse grid problems, in: Iterative Methods in Linear Algebra, edited by P. de Groen and R. Beauwens (IMACS, Elsevier, North Holland, 1992), pp. 263–281.
[3] M. Hegland, J. Garcke, and V. Challis, Linear Algebra and its Applications **420**(2–3), 249–275 (2007).