修士論文 要旨

Sparse grids capturing exponential decay and smoothness in Besov spaces (ベゾフ空間における関数の指数減衰と滑らかさを考慮したスパースグリッド)

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1 Introduction

Many problems in computational science and engineering involve high-dimensional approximations. Such functions appear when describing complex, nonlinear models and phenomena. In general, approximation of high-dimensional functions with linear combination of basis functions require a large number of basis functions. In some cases, the number of basis functions grows exponentially with respect to dimension. A method called sparse grid is known as a technique to mitigate this computational difficulty. The fundamental idea of sparse grids is to choose a fixed number of basis functions so that approximation error becomes as small as possible. Especially, smoothness and decay of functions are important to determine which basis functions should be used in sparse grids. In this study, by considering newly defined functions spaces called exponentially weighted Besov spaces with dominating smoothness $VB^{\delta,w}_{p,q}(\mathbb{R}^d)$, we give constructions of sparse grids capturing exponential decay and smoothness. Specifically, by obtaining wavelet characterization of $VB^{\delta,w}_{p,q}(\mathbb{R}^d)$, the sparse grids are obtained.

The motivation to consider sparse grids of this type is to solve eigenvalue problems of the following Hamilton operator H.

$$H := -\frac{1}{2}\sum_{\alpha=1}^{N}\Delta_i - \sum_{\alpha=1}^{N}\sum_{\nu=1}^{K}\frac{Z_\nu}{|x_i - a_\nu|} + \frac{1}{2}\sum_{\alpha,\beta=1 \alpha\neq\beta}^{N}\frac{1}{|x_i - x_j|}. \tag{1}$$

The Hamilton operator H, appears in the Schrödinger equation where multiple electrons interacts. The dimension of this system is $3N$, where N denotes the number of electrons. Thus, the dimension of problems are high when the number of electrons N are large. However, the eigenfunctions of above Hamilton operator H are known to have exponential decay and dominating mixed smoothness. There are rooms to improve complexity of eigenvalue problems of H by considering sparse grids capturing exponential decay and smoothness.

2 Exponentially weighted Besov spaces with dominating smoothness $VB^{\delta,w}_{p,q}(\mathbb{R}^d)$

Besov spaces $VB^{\delta,w}_{p,q}(\mathbb{R}^d)$, which are newly defined in this study, is an extension of normal Besov space $B^s_{p,q}(\mathbb{R}^d)$ and Besov space with mixed smoothness $MB^{\bar{s}}_{p,q}(\mathbb{R}^d)$. $VB^{\delta,w}_{p,q}(\mathbb{R}^d)$ is a weighted space whose weight function w increases or decreases exponentially at most, and has flexibility in smoothness. Especially, this flexibility includes smoothness of $B^s_{p,q}(\mathbb{R}^d)$, $MB^{\bar{s}}_{p,q}(\mathbb{R}^d)$ and their interpolations. Definitions of these two Besov spaces are given by the following quasinorms.

$$\left\| f \middle| B^s_{p,q}(\mathbb{R}^d) \right\| := \left(\sum_{j=0}^{\infty} 2^{sjq} \|\phi_j(\mathcal{D})f\|^q_{L^p} \right)^{1/q} \tag{2}$$

$$\left\| f \middle| MB^{\bar{s}}_{p,q}(\mathbb{R}^d) \right\| := \left(\sum_{\bar{j}\in\mathbb{N}_0^d} 2^{\bar{s}\cdot\bar{j}q} \|\Phi_{\bar{j}}(\mathcal{D})f\|^q_{L^p} \right)^{1/q} \tag{3}$$

where $\{\phi_j\}_{j\in\mathbb{N}_0}$ and $\{\Phi_{\bar{j}}\}_{\bar{j}\in\mathbb{N}_0^d}$ are dyadic resolutions of unity, and $\phi_j(\mathcal{D}) = \mathcal{F}^{-1}\phi_j\mathcal{F}$ and $\Phi_{\bar{j}}(\mathcal{D}) = \mathcal{F}^{-1}\Phi_{\bar{j}}\mathcal{F}$ ($\mathcal{F}$ is Fourier transform). Real numbers s in $B^s_{p,q}(\mathbb{R}^d)$ and $\bar{s}$ in $MB^{\bar{s}}_{p,q}(\mathbb{R}^d)$ are smoothness parameters, and control the convergence rate of L^p-norm of frequency components. These parameters are generalized by using norms δ on $\mathbb{N}_0^d$ instead. Exponentially weighted Besov spaces with dominating mixed smoothness $VB^{\delta,w}_{p,q}(\mathbb{R}^d)$ are defined by the following quasinorms.

$$\left\| f \middle| VB^{\delta,w}_{p,q}(\mathbb{R}^d) \right\| := \left(\sum_{j=0}^{\infty} 2^{\delta(\bar{j})q} \|\mathbf{\Psi}_{\bar{j}} * f\|^q_{L^w_p} \right)^{1/q}. \tag{4}$$

Note that, unlike quasinorms of non-weighted Besov spaces (2) and (3) , weighted L^p-norms are used in (4). Furthermore, in (4), the dyadic resolution of unity can not be used to define $VB^{\delta,w}_{p,q}(\mathbb{R}^d)$, thus different test functions $\{\mathbf{\Psi}_{\bar{j}}\}_{\bar{j}\in\mathbb{N}_0^d}$ are used. The reason for this is technical. For more details, see our paper.

3 Wavelet characterization of $VB^{\delta,w}_{p,q}(\mathbb{R}^d)$ and construction of sparse grids

Wavelet is a collection of orthogonal functions $\{\boldsymbol{\psi}_{\bar{j},\bar{m}}\}_{\bar{j}\in\mathbb{N}_0^d,\bar{m}\in\mathbb{Z}^d}$ which are derived from scaling and translation of only two functions. A function $f \in VB^{\delta,w}_{p,q}(\mathbb{R}^d)$ allow an expansion by wavelets.

$$f(x) = \sum_{\bar{j}\in\mathbb{N}_0^d}\sum_{\bar{m}\in\mathbb{Z}^d} \lambda_{\bar{j},\bar{m}}\boldsymbol{\psi}_{\bar{j},\bar{m}}(x)$$

where $\lambda_{\bar{j},\bar{m}}$ are real numbers and coefficients of $\boldsymbol{\psi}_{\bar{j},\bar{m}}$. Note that quasinorms of $\left\| f|VB^{\delta,w}_{p,q}(\mathbb{R}^d) \right\|$ are characterized by $\{\lambda_{\bar{j},\bar{m}}\}_{\bar{j}\in\mathbb{N}_0^d,\bar{m}\in\mathbb{Z}^d}$. Under certain assumptions, we prove the following relations(Theorem 3 in

Section 4.1).

$$A\|f\|_{VB^{\delta,w}_{p,q}} \le \left(\sum_{\vec{j}\in\mathbb{N}_0^d} 2^{\delta(\vec{j})q} \left\| \sum_{\bar{m}\in\mathbb{Z}^d} \lambda_{\bar{j},\bar{m}} \chi_{\bar{j},\bar{m}} \right\|^q_{L^p_w} \right)^{1/q} \le B\|f\|_{VB^{\delta,w}_{p,q}}$$

whre A and B are some positive constants, and $\chi_{\bar{j},\bar{m}}$ is an indicator function on $Q_{\bar{j},\bar{m}} = [\bar{m}/2^{\bar{j}}, (\bar{m}+\bar{1})/2^{\bar{j}}]$. This relation is called **wavelet characterization** of $VB^{\delta,w}_{p,q}(\mathbb{R}^d)$. Sparse grids on $VB^{\delta_1,w}_{p,q}(\mathbb{R}^d)$, which can capture exponential decay and mixed smoothness of function, can be easily derived from wavelet characterization of $VB^{\delta,w}_{p,q}(\mathbb{R}^d)$. Consider an approximation of f by the following finite wavelet expansion.

$$f \approx \sum_{\bar{j}\in\mathbb{N}_0^d} \sum_{\bar{m}\in\mathcal{M}_{\bar{j}}} \lambda_{\bar{j},\bar{m}} \psi_{\bar{j},\bar{m}} \tag{5}$$

where finite $\mathcal{M}_{\bar{j}}$ are non-empty so that summation in the left side is a finite summation. An approximation error of (5) can be estimated by wavelet characterization, i.e.,

$$\left\| f - \sum_{\bar{j}\in\mathbb{N}_0^d} \sum_{\bar{m}\in\mathcal{M}_{\bar{j}}} \lambda_{\bar{j},\bar{m}} \psi_{\bar{j},\bar{m}} \right\|_{VB^{\delta_1,1}_{p,q}} \lesssim \max_{\bar{j}\in\mathbb{N}_0^d} \left(2^{-(\delta_2(\bar{j})-\delta_1(\bar{j}))} \max_{\bar{m}\in\mathbb{Z}^d\setminus\mathcal{M}_{\bar{j}}} \left(\frac{|Q_{\bar{j},\bar{m}}|}{w(Q_{\bar{j},\bar{m}})} \right)^{1/p} \right) \times \|f\|_{VB^{\delta_2,w}_{p,q}}. \tag{6}$$

Sparse grids, a collection of sets $\{\mathcal{M}_{\bar{j}}\}_{\bar{j}\in\mathbb{N}_0^d}$, are obtained by minimizing approximation error in (6). Figure 1 shows an example of obtained sparse grids when dimension is 2.

4 Numerical Experiments

Consider the following problem to find minimum eigenvalue of H

$$H\Psi = E_{\min}\Psi$$

where $E_{\min}$ is a minimum eigenvalue, Ψ is a corresponding eigenfunctrion and H is 1-dimensional Hamiltonian defined by

$$H = -\frac{1}{2}\sum_{\alpha=1}^{N} \Delta_\alpha - \sum_{\alpha=1}^{N}\sum_{\nu=1}^{K} Z_\nu |x_\alpha - a_\nu| - \frac{1}{2}\sum_{\alpha,\beta=1\alpha\neq\beta}^{N} |x_i - x_j|$$

where $\Delta_\alpha = \frac{\partial^2}{\partial x^2_{\alpha,1}} + \cdots + \frac{\partial^2}{\partial x^2_{\alpha,d'}}$ and $d' = 1$. In this numerical experiments, we use sparse grids by setting $\delta_1 = 0$, $\delta_2(\bar{j}) = \theta|\bar{j}|_1 + |\bar{j}|_\infty$ and $p = 2$ in (6). These choices are due to the regularity results in [1]. Results of numerical experiments are shown in figure 2. Minimum eigenvalue problems are solved when $N = 2, 4, 6$. The results show we obtain asymptotic convergence of minimum eigenvalue $E_{\min}$ when $N = 2, 4$, but we can not reach asymptotic convergence when $N = 6$ with number of basis functions around two hundred thousand.

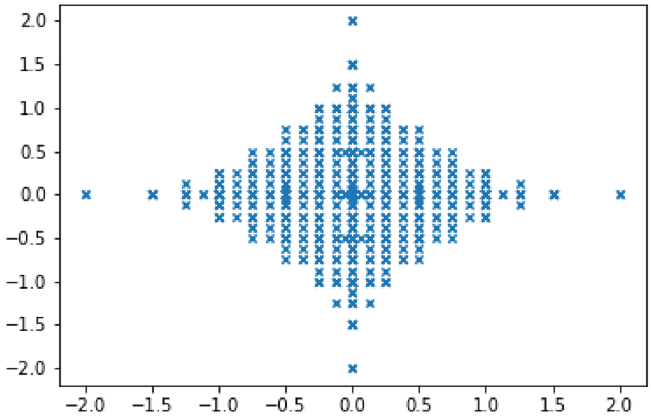

図 1. Plots of center of wavelets in 2 dimension 2when $w(x) = e^{b/p|x|_1}$, $b/p = 4$, $\delta_2(\cdot) = 0.25|\cdot|_1 + 0.75|\cdot|_\infty$, $\delta_1(\cdot) = 0$

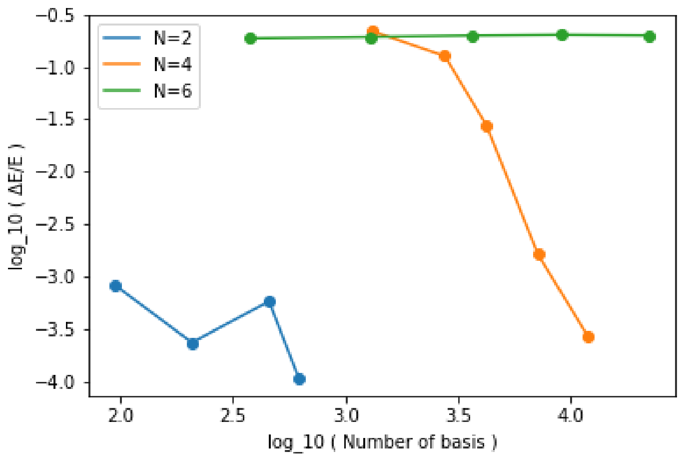

図 2. Results of eigenvalue of problems of H. $\Delta E/E$ is an absolute value of difference of successive eigenvalue over previous minimum eigenvalue.

参考文献

[1] Hans-Christian Kreusler and Harry Yserentant. The mixed regularity of electronic wave functions in fractional order and weighted sobolev spaces. *Numerische Mathematik*, 121(4):781–802, 2012.