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An analysis of wavelet frame based scattered data reconstruction

Jianbin Yang [a,b,*], Dominik Stahl [b], Zuowei Shen [b]

[a] Department of Mathematics, Hohai University, China
[b] Department of Mathematics, National University of Singapore, Singapore

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ABSTRACT

In real world applications many signals contain singularities, like edges in images. Recent wavelet frame based approaches were successfully applied to reconstruct scattered data from such functions while preserving these features. In this paper we present a recent approach which determines the approximant from shift invariant subspaces by minimizing an ℓ_1-regularized least squares problem which makes additional use of the wavelet frame transform in order to preserve sharp edges. We give a detailed analysis of this approach, i.e., how the approximation error behaves dependent on data density and noise level. Moreover, a link to wavelet frame based image restoration models is established and the convergence of these models is analyzed. In the end, we present some numerical examples, for instance how to apply this approach to handle coarse-grained models in molecular dynamics.

1. Introduction

The task of scattered data reconstruction is to determine a function that approximates a given set of unorganized points. It finds applications in various fields, for instance, terrain modeling, surface reconstruction and the numerical solution of partial differential equations, see e.g., [39]. Moreover, it can be used to approximate sparse range data [24], and it can be even applied to fit coarse-grained force functions in structural biology [34,31], as we will learn below.

Let $f : \mathbb{R}^d \to \mathbb{R}$ be a function, which usually is only known on some scattered data sites $\Xi = \{\xi_1, \xi_2, \dots, \xi_n\} \subset \mathbb{R}^d$ and additionally is disturbed by some noise, i.e., the given data is $y(\xi_i) = f(\xi_i) + \epsilon_i$ for $i = 1, 2, \dots, n$. The task of scattered data reconstruction is now to determine a function f^* from some function space V that approximates the noisy data $\{\xi_i, y(\xi_i)\}_{i=1}^n$. Most approaches determine the function f^* by solving a regularized least squares problem of the form

* Corresponding author at: Department of Mathematics, Hohai University, China.
E-mail addresses: jbyang@hhu.edu.cn (J. Yang), stahl@mathematik.uni-kl.de (D. Stahl), matzuows@nus.edu.sg (Z. Shen).

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$$\min_{g\in V}\sum_{i=1}^{n}(g(\xi_i)-y(\xi_i))^2+\Gamma(g)\ , \tag{1.1}$$

where the first term measures the fitting error while the regularization term $\Gamma(g)$ gives preferences to properties of the approximant f^*. It can for instance be chosen such that the roughness of f^* is penalized or such that f^* comes close to a piecewise continuous function, as we will present in this paper.

There are also several choices for the function space V in (1.1), often considered spaces are the Beppo-Levi space H^m, C^2 or as we will use in this paper, a shift invariant space

$$S^h(\phi):=closure\{\sum_{\alpha\in\mathbb{Z}^d}u(\alpha)\phi(\frac{\cdot}{h}-\alpha):u(\alpha)\in\mathbb{R}\ \text{ with }\ u(\alpha)=0\ \text{ for almost all }\ \alpha\in\mathbb{Z}^d\},$$

which is spanned by integer translates of just one compactly supported function ϕ that in turn is scaled by a $h>0$. Besides its structural simplicity shift invariant spaces have the beneficial property that for special choices of ϕ they provide good approximation orders to sufficiently smooth functions, see [25,26,29]. The compact support of ϕ also results in sparse system matrices which is of computational interest [29,40]. Such scaling functions ϕ are for instance B-splines, which in turn give rise to associated wavelet frame systems, as we discuss below.

Inspired by some recent wavelet frame based image restoration methodologies [7,36,24], we determine the approximating function $f^*\in S^h(\phi)$ by minimizing the functional

$$E^h(u):=\sum_{\xi\in\Xi}(\sum_{\alpha\in I}u(\alpha)\phi(\frac{\xi}{h}-\alpha)-y(\xi))^2+\nu\|\text{diag}(\lambda)\mathcal{W}u\|_{\ell_1(\mathbb{Z}^d)}\ , \tag{1.2}$$

where $u\in\ell_1(\mathbb{Z}^d)$, I is some properly chosen index set, ν is a positive parameter, $\mathcal{W}$ is the discrete framelet transform and diag(λ) is a diagonal matrix based on the vector λ which scales the different wavelet channels. The basic idea behind the regularization term in (1.2) is to make use of the interaction between the framelet transform and the ℓ_1-norm. It is a known fact that the wavelet coefficient sequence of a signal, which is sampled from a piecewise smooth function, is sparse. Furthermore, because of the ℓ_1-norm, the regularization term $\|\text{diag}(\lambda)\mathcal{W}u\|_{\ell_1}$ gives preference to a solution u whose wavelet coefficient sequence is sparse, and to keep the singularities of functions. This property makes the approach (1.2) predestined for applications like range data approximation, as it is demonstrated in [24]. However in [24] the location of the scattered data sites Ξ is only considered on regular grids, i.e., scaled subsets of $\mathbb{Z}^2$ and no error analysis of the method is given.

The main focus of this paper is to extend this to bounded subsets $\Omega\subset\mathbb{R}^d$ and to give a proper approximation analysis to the approach connected to (1.2), i.e., let $f\in W_1^k$, given some scattered data $y(\xi_i)=f(\xi_i)+\epsilon_i$ with $\xi_i\in\Xi\subset\Omega$ and some noise ϵ_i, how does $\|f^*-f\|_{L_p(\Omega)}$ behave dependent on the data density, the noise level and the dilation h, where $f^*:=\sum_\alpha u^*(\alpha)\phi(\cdot/h-\alpha)$ with $u^*=\arg\min_u E^h(u)$ being the minimizer of (1.2). Similar has been considered in [29] for the model

$$\min_{g\in S^h(\phi)}\sum_{\xi\in\Xi}(g(\xi)-y(\xi))^2+\nu|g|^2_{H^m}\ ,$$

whose minimizer can be seen as an approximation to the thin plate smoothing spline. Hence gives a smooth approximation to the scattered data, meaning that discontinuities are not displayed very well. Additionally in numerical considerations the regularization term $|g|^2_{H^m}$ has to be discretized, but no approximation result is given for this discrete case. This is another advantage of the approach (1.2), because no discretization of the regularization term is needed as it is already in discrete form and so the approximation results which we present stay valid. Since in real world applications many signals contain singularities, the approach (1.2) finds various applications.

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