# Greedy Criterion in Orthogonal Greedy Learning

Lin Xu, Shaobo Lin, Jinshan Zeng, Xia Liu and Zongben Xu

Abstract—Orthogonal greedy learning (OGL) is a stepwise learning scheme that starts with selecting a new atom from a specified dictionary via the steepest gradient descent (SGD) and then builds the estimator through orthogonal projection. In this paper, we find that SGD is not the unique greedy criterion and introduce a new greedy criterion, called " $\delta$ -greedy threshold" for learning. Based on the new greedy criterion, we derive an adaptive termination rule for OGL. Our theoretical study shows that the new learning scheme can achieve the existing (almost) optimal learning rate of OGL. Plenty of numerical experiments are provided to support that the new scheme can achieve almost optimal generalization performance, while requiring less computation than OGL.

Index Terms—Supervised learning, greedy algorithms, orthogonal greedy learning, greedy criterion, generalization capability.

#### I. INTRODUCTION

UPERVISED learning focuses on synthesizing a function to approximate an underlying relationship between inputs and outputs based on finitely many input-output samples. Commonly, a system tackling supervised learning problems is called as a learning system. A standard learning system usually comprises a hypothesis space, an optimization strategy and a learning algorithm. The hypothesis space is a family of parameterized functions providing a candidate set of estimators, the optimization strategy formulates an optimization problem to define the estimator based on samples, and the learning algorithm is an inference procedure that numerically solves the optimization problem.

Dictionary learning is a special learning system, whose hypothesis spaces are linear combinations of atoms in some given dictionaries. Here, the dictionary denotes a family of base learners [41]. For such type hypothesis spaces, many regularization schemes such as the bridge estimator [1], ridge estimator [22] and Lasso estimator [44] are common used optimization strategies. When the scale of dictionary is moderate (i.e., about hundreds of atoms), these optimization strategies can be effectively realized by various learning algorithms such as the regularized least squares algorithms [47], iterative thresholding algorithms [15] and iterative re-weighted algorithms [16]. However, when presented large input dictionary, a large portion of the aforementioned learning algorithms are time-consuming and even worse, they may cause the sluggishness of the corresponding learning systems.

Greedy learning or, more specifically, learning by greedy type algorithms, provides a possible way to circumvent the drawbacks of regularization methods [2]. Greedy algorithms are stepwise inference processes that start from a null model and solve heuristically the problem heuristically of making the locally optimal choice at each step with the hope of finding a global optimum. Within moderate number of iterations, greedy algorithms possess charming computational advantage compared with the regularization schemes [41]. This property triggers avid research activities of greedy algorithms in signal processing [14], [26], [45], inverse problems [19], [46], sparse approximation [18], [43] and machine learning [2], [9], [29].

## A. Motivations of greedy criteria

Orthogonal greedy learning (OGL) is a special greedy learning strategy. It selects a new atom based on SGD in each iteration and then constructs an estimator through orthogonal projecting to subspaces spanned by the selected atoms. It is well known that SGD needs to traverse the whole dictionary, which leads to an insufferable computational burden when the scale of dictionary is large. Moreover, as the samples are noised, the generalization capability of OGL is sensitive to the number of iterations. In other words, due to the SGD criterion, a slight turbulence of the number of atoms may lead to a great change of the generalization performance.

To overcome the above problems of OGL, a natural idea is to re-regulate the criterion to choose a new atom by taking the "greedy criterion" issue into account. The Fig. 1 is an intuitive description to quantify the greedy criterion, where  $r_k$  represents the residual at the k-th iteration, g is an arbitrary atom from the dictionary and  $\theta$  is the included angle between  $r_k$  and g. In Fig. 1 (a), both  $r_k$  and g are normalized to the unit ball due to the greedy criterion focusing on the orientation rather than magnitude. The cosine of the angle  $\theta$  (cosine similarity) is used to quantify the greedy criterion. As shown in Fig. 1 (b), the atom  $g_k$  possessing the smallest  $\theta$  is regarded to be the greediest one at each iteration in OGL.

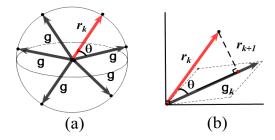


Fig. 1: An intuitive description of the greedy criterion. (a) Normalize the current residual  $r_k$  and atoms g to the unit ball. (b) The atom  $g_k$  possessing the smallest  $\theta$  is regarded to be the greediest one at each iteration.

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Since the greedy criterion can be quantified by the cosine similarity, a preferable way to circumvent the aforementioned problems of OGL is to weaken the level of greed by thresholding the cosine similarity. In particular, other than traversing the dictionary, we can select the first atom satisfying the thresholding condition. Such a method essentially reduces the computation cost of OGL and makes the learning process more

#### B. Our contributions

stable.

Different from other three issues, the "greedy criterion" issue, to the best of our knowledge, has not been noted for the learning purpose. The aim of the present paper is to reveal the importance and necessity of studying the "greedy criterion" issue in OGL. The main contributions can be summarized as follows.

- We argue that SGD is not the unique criterion for OGL. There are many other greedy criteria in greedy learning, which possess similar learning performance as SGD.
- We use a new greedy criterion called the " $\delta$ -greedy threshold" to quantify the level of greed in OGL. Although a similar criterion has already been used in greedy approximation [42], the novelty of translating it into greedy learning is that using this criterion can significantly accelerate the learning process. We can also prove that, if the number of iteration is appropriately specified, then OGL with the " $\delta$ -greedy threshold" can reach the existing (almost) optimal learning rate of OGL [2].
- Based on the " $\delta$ -greedy threshold" criterion, we propose an adaptive terminate rule for OGL and then provide a complete learning system called  $\delta$ -thresholding orthogonal greedy learning ( $\delta$ -TOGL). Different from classical termination rules that devote to searching the appropriate number of iterations based on the bias-variance balance principle [2], [49], our study implies that the balance can also be attained through setting a suitable greedy threshold. This phenomenon reveals the essential importance of the "greedy criterion" issue. We also present the theoretical justification of  $\delta$ -TOGL.
- We carefully analyze the generalization performance and computation cost of  $\delta$ -TOGL, compared with other popular learning strategies such as the pure greedy learning (PGL) [2], [41], OGL, regularized least squares (RLS) [24] and fast iterative shrinkage-thresholding algorithm (FISTA) [4] through plenty of numerical studies. The main advantage of  $\delta$ -TOGL is that it can reduce the computational cost without sacrificing the generalization capability. In many applications, it can learn hundreds of times faster than conventional methods.

#### C. Organization

The rest of the paper is organized as follows. In Section 2, we present a brief introduction of statistical learning theory and greedy learning. In Section 3, we introduce the " $\delta$ -greedy threshold" criterion in OGL and provide its feasibility justification. In Section 4, based on the " $\delta$ -greedy threshold" criterion, we propose an adaptive termination rule and the corresponding  $\delta$ -TOGL system. The theoretical feasibility of the  $\delta$ -TOGL system is also given in this section. In Section

5, we present numerical simulation experiments to verify our arguments. In Section 6,  $\delta$ -TOGL is tested with real-world data. In Section 7, we provide the detailed proofs of the main results. Finally, the conclusion is drawn in the last section.

#### II. PRELIMINARIES

In this section, we present some preliminaries to serve as the basis for the following sections.

#### A. Statistical learning theory

Suppose that the samples  $\mathbf{z}=(x_i,y_i)_{i=1}^m$  are drawn independently and identically from  $Z:=X\times Y$  according to an unknown probability distribution  $\rho$  which admits the decomposition

$$\rho(x,y) = \rho_X(x)\rho(y|x). \tag{II.1}$$

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Let  $f: X \to Y$  be an approximation of the underlying relation between the input and output spaces. A commonly used measurement of the quality of f is the generalization error, defined by

$$\mathcal{E}(f) := \int_{Z} (f(x) - y)^{2} d\rho, \tag{II.2}$$

which is minimized by the regression function [10]

$$f_{\rho}(x) := \int_{Y} y d\rho(y|x). \tag{II.3}$$

The goal of learning is to find a best approximation of the regression function  $f_{\rho}$ .

Let  $L^2_{\rho_X}$  be the Hilbert space of  $\rho_X$  square integrable functions on X, with norm  $\|\cdot\|_{\rho}$ . It is known that, for every  $f\in L^2_{\rho_X}$ , it holds that

$$\mathcal{E}(f) - \mathcal{E}(f_{\rho}) = \|f - f_{\rho}\|_{\rho}^{2}. \tag{II.4}$$

Without loss of generality, we assume  $y \in [-M, M]$  almost surely. Thus, it is reasonable to truncate the estimator to [-M, M]. That is, if we define

$$\pi_M u := \left\{ \begin{array}{ll} u, & \text{if } |u| \leq M \\ M \text{sign}(u), & \text{otherwise} \end{array} \right. \tag{II.5}$$

as the truncation operator, where sign(u) represents the sign function of u, then

$$\|\pi_M f_{\mathbf{z}} - f_{\rho}\|_{\rho}^2 \le \|f_{\mathbf{z}} - f_{\rho}\|_{\rho}^2.$$
 (II.6)

## B. Greedy learning

Four most important elements of greedy learning are dictionary selection, greedy criterion, iterative strategy and termination rule. This is essentially different from greedy approximation which focuses only on dictionary selection and iterative format issues [41]. Greedy learning concerns not only the approximation capability, but also the cost, such as the model complexity, which should pay to achieve a specified approximation accuracy. In a nutshell, greedy learning can be regarded as a four-issue learning scheme.

• Dictionary selection: this issue devotes to selecting a suitable dictionary for a given learning task. As a classical

topic of greedy approximation, there are a great deal of dictionaries available to greedy learning. Typical examples include the greedy basis [41], quasi-greedy basis [40], redundant dictionary [17], orthogonal basis [37], kernel-based sample dependent dictionary [8], [29] and tree [21].

- Greedy criterion: this issue regulates the criterion to choose a new atom from the dictionary in each greedy step. Besides the widely used steepest gradient descent (SGD) method [17], there are also many methods such as the weak greedy [38], thresholding greedy [41] and super greedy [31] to quantify the greedy criterion for approximation purpose. However, to the best of our knowledge, only the SGD criterion is employed in greedy learning, since all the results in greedy approximation [31], [38], [41] imply that SGD is superior to other criteria.
- Iterative format: this issue focuses on how to define a new estimator based on the selected atoms. Similar to the "dictionary selection", the "iterative format" issue is also a classical topic in greedy approximation. There are several types of iterative schemes [41]. Among these, three most commonly used iterative schemes are pure greedy [28], orthogonal greedy [17] and relaxed greedy formats [42]. Each iterative format possesses its own pros and cons [40], [41]. For instance, compared with the orthogonal greedy format, pure and relaxed greedy formats have benefits in computation but suffer from either low convergence rate or small applicable scope.
- Termination rule: this issue depicts how to terminate the learning process. The termination rule is regarded as the main difference between greedy approximation and learning, which has been recently studied [2], [8], [29], [49]. For example, Barron et al. [2] proposed an  $l^0$ -based complexity regularization strategy as the termination rule, and Chen et al. [8] provided an  $l^1$ -based adaptive termination rule.

Let H be a Hilbert space endowed with norm  $\|\cdot\|_H$  and inner product  $\langle\cdot,\cdot\rangle_H$ . Let  $\mathcal{D}=\{g\}_{g\in\mathcal{D}}$  be a given dictionary satisfying  $\sup_{g\in D,x\in X}|g(x)|\leq 1$ . Denote  $\mathcal{L}_1=\{f:f=\sum_{g\in D}a_gg\}$  as a Banach space endowed with the norm

$$||f||_{\mathcal{L}_1} := \inf_{\{a_g\}_{g \in \mathcal{D}}} \left\{ \sum_{g \in \mathcal{D}} |a_g| : f = \sum_{g \in \mathcal{D}} a_g g \right\}.$$
 (II.7)

There exist several types of greedy algorithms [40]. The three most commonly used are the pure greedy algorithm (PGA) [28], orthogonal greedy algorithm (OGA) [17] and relaxed greedy algorithm (RGA) [42]. These algorithms initialize with  $f_0 := 0$ . The new approximation  $f_k$   $(k \ge 1)$  is defined based on  $r_{k-1} := f - f_{k-1}$ . In OGA,  $f_k$  is defined by

$$f_k = P_{V_{\mathbf{z},k}} f, \tag{II.8}$$

where  $P_{V_{\mathbf{z},k}}$  is the orthogonal projection onto the space  $V_{\mathbf{z},k} = \operatorname{span}\{g_1,\ldots,g_k\}$  and  $g_k$  is defined as

$$g_k = \arg\max_{g \in \mathcal{D}} |\langle r_{k-1}, g \rangle_H|.$$
 (II.9)

Given  $\mathbf{z} = (x_i, y_i)_{i=1}^m$ , the empirical inner product and norm are defined by

$$\langle f, g \rangle_m := \frac{1}{m} \sum_{i=1}^m f(x_i) g(x_i), \tag{II.10}$$

and

$$||f||_m^2 := \frac{1}{m} \sum_{i=1}^m |f(x_i)|^2.$$
 (II.11)

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Setting  $f_{\mathbf{z}}^0 = 0$ , the four aforementioned issues are attended in OGL as follows:

- Dictionary selection: Select a suitable dictionary  $\mathcal{D}_n := \{g_1, \dots, g_n\}.$
- · Greedy criterion:

$$g_k = \arg \max_{g \in \mathcal{D}_n} |\langle r_{k-1}, g \rangle_m|.$$
 (II.12)

• Iteration format:

$$f_{\mathbf{z}}^k = P_{V_{\mathbf{z},k}} f, \tag{II.13}$$

where  $P_{V_{\mathbf{z},k}}$  is the orthogonal projection onto  $V_{\mathbf{z},k} = \operatorname{span}\{g_1,\ldots,g_k\}$  in the metric of  $\langle\cdot,\cdot\rangle_m$ .

• Termination rule: Terminate the learning process when *k* satisfies a certain assumption.

#### III. GREEDY CRITERION IN OGL

Given a real functional  $V: H \to \mathbf{R}$ , the Fréchet derivative of V at  $f, V'_f: H \to \mathbf{R}$  is a linear functional such that for  $h \in H$ .

$$\lim_{\|h\|_{H} \to 0} \frac{|V(f+h) - V(f) - V'_{f}(h)|}{\|h\|_{H}} = 0, \quad (III.1)$$

and the gradient of V as a map  $\operatorname{grad} V: H \to H$  is defined by

$$\langle \operatorname{grad} V(f), h \rangle_H = V'_f(h), \text{ for all } h \in H.$$
 (III.2)

The greedy criterion adopted in Eq.(II.12) is to find  $g_k \in \mathcal{D}_n$  such that

$$\langle -\operatorname{grad}(A_m)(f_{\mathbf{z}}^{k-1}), g_k \rangle = \sup_{g \in \mathcal{D}_n} \langle -\operatorname{grad}(A_m)(f_{\mathbf{z}}^{k-1}), g \rangle,$$
(III.3)

where  $A_m(f) = \sum_{i=1}^m |f(x_i) - y_i|^2$ . Therefore, the classical greedy criterion is based on the steepest gradient descent (SGD) of  $r_{k-1}$  with respect to the dictionary  $\mathcal{D}_n$ . By normalizing the residual  $r_k$ ,  $k=0,1,2,\ldots,n$ , greedy criterion in Eq.(II.12) means to search  $g_k$  satisfying

$$g_k = \arg\max_{g \in \mathcal{D}_n} \frac{|\langle r_{k-1}, g \rangle_m|}{\|r_{k-1}\|_m}.$$
 (III.4)

Geometrically, the current  $g_k$  minimizes the angle between  $r_{k-1}/\|r_{k-1}\|_m$  and g, which is depicted in Fig. 1.

Recalling the definition of OGL, it is not difficult to verify that the angles satisfy

$$|\cos \theta_1| \le |\cos \theta_2| \le \dots \le |\cos \theta_k| \le \dots \le |\cos \theta_n|,$$
(III.5)

or

or
$$\frac{|\langle r_0, g_1 \rangle_m|}{\|r_0\|_m} \ge \dots \ge \frac{|\langle r_{k-1}, g_k \rangle_m|}{\|r_{k-1}\|_m} \ge \dots \ge \frac{|\langle r_{n-1}, g_n \rangle_m|}{\|r_{n-1}\|_m}, \tag{III.6}$$

since  $\frac{|\langle r_{k-1}, g_k \rangle_m|}{\|r_{k-1}\|_m} = |\cos \theta_k|$ . If the algorithm stops at the k-th iteration, then there exists a threshold  $\delta \in [|\cos \theta_k|, |\cos \theta_{k+1}|]$  to quantify whether another atom should be added to construct the final estimator. To be detailed, if

$$\frac{|\langle r_{k-1}, g_k \rangle_m|}{\|r_{k-1}\|_m} > \delta. \tag{III.7}$$

If there is no  $g_k$  satisfying Eq. (III.7), then the algorithm terminates. We call the greedy criterion Eq. (III.7) as the " $\delta$ -greedy threshold" criterion. In practice, the number of "active atom" is usually not unique. We can choose the first "active atom" satisfied Eq. (III.7) at each greedy iteration to accelerate the algorithm. Once the "active atom" is selected, then the algorithm goes to the next greedy iteration and the "active atom" is redefined.

Through such a greedy-criterion, we can develop a new orthogonal greedy learning scheme, called thresholding orthogonal greedy learning (TOGL). The two corresponding elements of TOGL can be reformulated as follows:

- Greedy definition: Let  $g_k$  be an arbitrary (or the first) atom from  $\mathcal{D}_n$  satisfying Eq. (III.7).
- Termination rule: Terminate the learning process either there is no atom satisfying Eq. (III.7) or k satisfies a certain assumption.

Without considering the termination rule, the classical greedy criterion Eq. (II.12) in OGL always selects the greediest atom at each greedy iteration. However, Eq. (III.7) slows down the speed of gradient descent and therefore may conduct a more flexible model selection strategy. According to the bias and variance balance principle [13], the bias decreases while the variance increases as a new atom is selected to build the estimator. If a lower-correlation atom is added, then the bias decreases slower and the variance also increases slower. Then, the balance can be achieved in TOGL within a more gradual flavor than OGL. Moreover, Eq. (III.7) also provides a terminate condition that if all atoms, g, in  $\mathcal{D}_n$  satisfy

$$\frac{|\langle r_{k-1}, g \rangle_m|}{\|r_{k-1}\|_m} \le \delta, \tag{III.8}$$

then the algorithm terminates. The termination rule concerning k in TOGL is necessary and is used to avoid certain extreme cases in practice. Indeed, using only the terminate condition Eq. (III.8) may drive the algorithm to select all atoms from  $\mathcal{D}_n$ . As Fig. 2 shows, if the target function f is almost orthogonal to the space spanned by the dictionary and atoms in the dictionary are almost linear dependent, then the selected  $\delta$  should be too small to distinguish which is the "active atom". Consequently, the corresponding learning scheme selects all atoms of dictionary and therefore degrades the generalization capability of OGL.

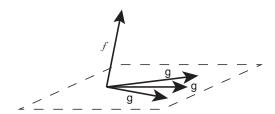


Fig. 2: The necessity of termination rule concerning k in TOGL.

Now we present a theoretical assessment of TOGL. At first, we give a few notations and concepts, which will be used in the rest part of the paper. For r>0, the space  $\mathcal{L}^r_{1,\mathcal{D}_n}$  is defined to be the set of all functions f such that, there exists a  $h\in\operatorname{span}\{\mathcal{D}_n\}$  satisfying

$$||h||_{\mathcal{L}_1(\mathcal{D}_n)} \le \mathcal{B}$$
, and  $||f - h|| \le \mathcal{B}n^{-r}$ , (III.9)

where  $\|\cdot\|$  denotes the uniform norm for the continuous function space C(X). The infimum of all  $\mathcal B$  satisfying Eq. (III.9) defines a norm (for f) on  $\mathcal L^r_{1,\mathcal D_n}$ . The Eq. (III.9) defines an interpolation space and is a natural assumption for the regression function in greedy learning [2]. This assumption has already been adopted to analyze the learning capability of greedy learning [2], [29], [49]. The Theorem III.1 illustrates the performance of TOGL and consequently, reveals the feasibility of the greedy criterion in Eq. (III.7).

**Theorem III.1.** Let 0 < t < 1,  $0 < \delta \le 1/2$ , and  $f_{\mathbf{z}}^{k,\delta}$  be the estimator deduced by TOGL. If  $f_{\rho} \in \mathcal{L}_{1,\mathcal{D}_{n}}^{r}$ , then there exits a  $k^{*} \in \mathbf{N}$  such that

$$\mathcal{E}(\pi_M f_{\mathbf{z}}^{k^*,\delta}) - \mathcal{E}(f_{\rho}) \le C\mathcal{B}^2((m\delta^2)^{-1}\log m\log\frac{1}{\delta}\log\frac{2}{t} + \delta^2 + n^{-2r})$$

holds with probability at least 1 - t, where C is a positive constant depending only on d and M.

If  $\delta = \mathcal{O}(m^{-1/4})$ , and the size of dictionary, n, is selected to be large enough, i.e.,  $n \geq \mathcal{O}(m^{\frac{1}{4r}})$ , then Theorem III.1 shows that the generalization error of  $\pi_M f_{\mathbf{z}}^{k^*,\delta}$  is asymptotic to  $\mathcal{O}(m^{-1/2}(\log m)^2)$ . Up to a logarithmic factor, this bound is the same as that in [2] and is the "record" of OGL. This implies that weakening the level of greed in OGL is a feasible way to avoid traversing the dictionary. It should also be pointed out that different from OGL [2], there are two parameters, k and  $\delta$ , in TOGL. Therefore, Theorem III.1 only presents a theoretical verification that introducing the " $\delta$ -greedy threshold" to measure the level of greed does not essentially degrade the generalization capability of OGL. Taking the practical applications into account, eliminating the condition concerning k in the termination rule is crucial. This is the scope of the following section, where an adaptive termination rule with respect to  $\delta$  is presented.

#### IV. $\delta$ -thresholding orthogonal greedy learning

In the previous section, we developed a new greedy learning scheme called as thresholding orthogonal greedy learning (TOGL) and theoretically verified its feasibility. However, there are two main parameters (i.e., the value of threshold  $\delta$  and iteration k) should be simultaneously fine-tuned. It puts more pressure on parameter selection, which may dampen the spirits of practitioners. Given this, we further propose an adaptive termination rule only based on the value of threshold. Notice that, the value  $\|r_{k-1}\|_m/\|y(\cdot)\|_m$  becomes smaller and smaller along the selection of more and more "active" atoms, where  $y(\cdot)$  is a function satisfying  $y(x_i)=y_i, i=1,\ldots,m$ . Then, an advisable terminate condition is to use  $\delta$  to quantify  $\|r_{k-1}\|_m/\|y(\cdot)\|_m$ . Therefore, we append another terminate condition as

$$||r_{k-1}||_m \le \delta ||y(\cdot)||_m \tag{IV.1}$$

to replace the previous terminate condition concerning k in TOGL. Based on it, a new termination rule can be obtained:

• Termination rule: Terminate the learning process if either Eq. (IV.1) holds or there is no atom satisfying Eq. (III.7). That is:

$$\max_{g \in \mathcal{D}_n} |\langle r_k, g \rangle_m| \le \delta ||r_k||_m \text{ or } ||r_k||_m \le \delta ||f||_m. \text{ (IV.2)}$$

For such a change, we present a new learning system named the  $\delta$ -thresholding orthogonal greedy learning ( $\delta$ -TOGL) as the Algorithm 1.

## Algorithm 1 $\delta$ -TOGL

## Step 1 (Initialization):

Given data  $\mathbf{z} = (x_i, y_i)_{i=1}^m$  and dictionary  $\mathcal{D}_n$ .

Given a proper greedy threshold  $\delta$ .

Set initial estimator  $f_0 = 0$  and iteration k := 0.

## Step 2 ( $\delta$ -greedy threshold):

Select  $g_k$  be an arbitrary atom from  $\mathcal{D}_n$  satisfying

$$\frac{|\langle r_{k-1}, g_k \rangle_m|}{\|r_{k-1}\|_m} > \delta.$$

## **Step 3 (Orthogonal projection):**

Let  $V_{\mathbf{z},k} = \operatorname{Span}\{g_1, \dots, g_k\}$ . Compute  $f_{\mathbf{z}}^{\delta}$  as:

$$f_{\mathbf{z}}^{\delta} = P_{\mathbf{z}, V_{\mathbf{z}, k}}(y).$$

The residual:  $r_k := y - f_{\mathbf{z}}^{\delta}$ , where  $P_{\mathbf{z},V_{\mathbf{z},k}}$  is the orthogonal projection onto space  $V_{\mathbf{z},k}$  in the criterion of  $\langle \cdot, \cdot \rangle_m$ .

#### Step 4 (Termination rule):

If termination rule satisfied as:

$$\max_{g \in \mathcal{D}_n} |\langle r_k, g \rangle_m| \le \delta ||r_k||_m \text{ or } ||r_k||_m \le \delta ||f||_m,$$

then the algorithm terminates and outputs final estimator  $f_{\mathbf{z}}^{\delta}$ . Otherwise, turn to Step 2 and k := k + 1.

The implementation of OGL requires traversing the dictionary, which has a complexity of  $\mathcal{O}(mn)$ . Inverting a  $k \times k$  matrix in orthogonal projection has a complexity of  $\mathcal{O}(k^3)$ . Thus, the kth iteration of OGL has a complexity of  $\mathcal{O}(mn+k^3)$ . In Step 2 of  $\delta$ -TOGL,  $g_k$  is an arbitrary atom from  $\mathcal{D}_n$  satisfying the " $\delta$ -greedy threshold" condition. It motivates us to select the first atom from  $\mathcal{D}_n$  satisfying Eq. (III.7). Then the complexity of  $\delta$ -TOGL is smaller than  $\mathcal{O}(mn+k^3)$ . In fact, it usually requires a complexity of  $\mathcal{O}(m+k^3)$ , and gets a complexity

of  $\mathcal{O}(mn+k^3)$  only for the worst case.  $\delta$ -TOGLR essentially reduces the complexity of OGL, especially when n is large. The memory requirements of OGL and  $\delta$ -TOGL are  $\mathcal{O}(mn)$ .

The following theorem shows that if  $\delta$  is appropriately tuned, then the  $\delta$ -TOGL estimator  $f_{\mathbf{z}}^{\delta}$  can realize the (almost) optimal generalization capability of OGL and TOGL.

**Theorem IV.1.** Let 0 < t < 1,  $0 < \delta \le 1/2$ , and  $f_{\mathbf{z}}^{\delta}$  be defined in Algorithm 1. If  $f_{\rho} \in \mathcal{L}_{1,\mathcal{D}_{n}}^{r}$ , then the inequality

$$\mathcal{E}(\pi_M f_{\mathbf{z}}^{\delta}) - \mathcal{E}(f_{\rho}) \le C\mathcal{B}^2((m\delta^2)^{-1}\log m \log \frac{1}{\delta} \log \frac{2}{t} + \delta^2 + n^{-2r})$$

holds with probability at least 1 - t, where C is a positive constant depending only on d and M.

If  $n \geq \mathcal{O}(m^{\frac{1}{4r}})$  and  $\delta = \mathcal{O}(m^{-1/4})$ , then the learning rate in Theorem IV.1 asymptotically equals to  $\mathcal{O}(m^{-1/2}(\log m)^2)$ , which is the same as that of Theorem III.1. Therefore, Theorem IV.1 implies that using Eq. (IV.1) to replace the terminate condition concerning k is theoretically feasible. The most important highlight of Theorem IV.1 is that it provides a totally different way to circumvent the overfitting phenomenon of OGL. The termination rule is crucial for OGL, but designing an effective termination rule is a tricky problem. All the aforementioned studies [2], [8], [49] of the termination rule attempted to design a termination rule by controlling the number of iterations directly. Since the generalization capability of OGL is sensitive to the number of iterations, the results are at times inadequate. The termination rule employed in the present paper is based on the study of the "greedycriterion" issue of greedy learning. Theorem IV.1 shows that, besides controlling the number of iterations directly, setting a greedy threshold to redefine the greedy criterion can also conduct an effective termination rule. Theorem IV.1 implies that this new termination rule theoretically works as well as others. Furthermore, when compared with k in OGL, the generalization capability of the  $\delta$ -TOGL is stable to  $\delta$ , since the new criterion slows down the changes of bias and variance.

## V. SIMULATION VERIFICATIONS

In this section, a series of simulations are carried out to verify our theoretical assertions. Firstly, we introduce the simulation settings, including the data sets, dictionary, greedy criteria and experimental environment. Secondly, we analyze the relationship between the greedy criteria and generalization performance in orthogonal greedy learning (OGL) and demonstrate that steepest gradient descent (SGD) is not the unique greedy criterion. Thirdly, we present a performance comparison of different greedy criteria and illustrate the " $\delta$ -greedy threshold" is feasible. Fourthly, we empirically study the performance of  $\delta$ -thresholding orthogonal greedy learning ( $\delta$ -TOGL) and justify the feasibility of it. Finally, we compare  $\delta$ -TOGL with other widely used dictionary-based learning methods and show it is a promising learning scheme.

## A. Simulation settings

Throughout the simulations, let  $\mathbf{z} = \{(x_i, y_i)\}_{i=1}^{m_1}$  be the training samples with  $\{x_i\}_{i=1}^{m_1}$  being drawn independently and

identically according to the uniform distribution on  $[-\pi, \pi]$  and  $y_i = f_{\rho}(x_i) + \mathcal{N}(0, \sigma^2)$ , where

$$f_{\rho}(x) = \frac{\sin x}{x}, \quad x \in [-\pi, \pi].$$

Four levels of noise:  $\sigma_1 = 0.1$ ,  $\sigma_2 = 0.5$ ,  $\sigma_3 = 1$  and  $\sigma_4 = 2$  are used in the simulations. The learning performance (in terms of root mean squared error (RMSE)) of different algorithms are then tested by applying the resultant estimators to the test set  $\mathbf{z}_{test} = \{(x_i^{(t)}, y_i^{(t)})\}_{i=1}^{m_2}$ , which is similarly generated as  $\mathbf{z}$  but with a promise that  $y_i$  are taken to be  $y_i^{(t)} = f_\rho(x_i^{(t)})$ .

In each simulation, we use the Gaussian radial basis function (RBF) [12] to build up the dictionary:

$$\left\{e^{-\|x-t_i\|^2/\eta^2}: i=1,\ldots,n\right\},$$

where  $\{t_i\}_{i=1}^n$  are drawn according to the uniform distribution in  $[-\pi, \pi]$ . Since the aim of each simulation is to compare  $\delta$ -TOGL with other learning methods on the same dictionary, we just set  $\eta = 1$  throughout the simulations.

We use four different criteria to select the new atom in each greedy iteration:

$$\begin{split} g_k &:= \arg\max_{g \in \mathcal{D}_n} |\langle r_{k-1}, g \rangle_m|, \\ g_k &:= \arg\operatorname*{second}\max_{g \in \mathcal{D}_n} |\langle r_{k-1}, g \rangle_m|, \\ g_k &:= \operatorname*{arg}\operatorname*{third}\max_{g \in \mathcal{D}_n} |\langle r_{k-1}, g \rangle_m|, \end{split}$$

and

 $g_k$  randomly selected from  $\mathcal{D}_n$ .

Here,  $\arg\operatorname{second}\max$  and  $\arg\operatorname{third}\max$  mean the values of  $|\langle r_{k-1},g\rangle_m|$  reach the second and third largest values, respectively. Randomly selected means to randomly select  $g_k$  from the dictionary. We use four abbreviations OGL1, OGL2, OGL3 and OGLR to to denote the corresponding learning schemes, respectively.

Let  $\mathcal{D}_{n,k,\delta}$  be the set of atoms of  $\mathcal{D}_n$  satisfying  $\frac{|\langle r_{k-1}, g_k \rangle_m|}{\|r_{k-1}\|_m} > \delta$ . Four corresponding criteria are employed as following:

$$\begin{split} g_k &:= \arg\max_{g \in \mathcal{D}_{n,k,\delta}} |\langle r_{k-1}, g \rangle_m|, \\ g_k &:= \arg\operatorname*{second}\max_{g \in \mathcal{D}_{n,k,\delta}} |\langle r_{k-1}, g \rangle_m|, \\ g_k &:= \operatorname*{arg}\operatorname*{third}\max_{g \in \mathcal{D}_{n,k,\delta}} |\langle r_{k-1}, g \rangle_m|, \end{split}$$

and

$$g_k = \text{First}(D_{n,k,\delta}).$$

Here  $\operatorname{First}(D_{n,k,\delta})$  denotes the first atom of  $\mathcal{D}_n$  satisfying  $\frac{|\langle r_{k-1}, g_k \rangle_m|}{\|r_{k-1}\|_m} > \delta$ . We also use TOGL1 (or  $\delta$ -TOGL1), TOGL2 (or  $\delta$ -TOGL2), TOGL3 (or  $\delta$ -TOGL3) and TOGLR (or  $\delta$ -TOGLR) to denote the corresponding algorithms.

All numerical studies are implemented by MATLAB R2015a on a Windows personal computer with Core(TM) i7-3770 3.40GHz CPUs and RAM 16.00GB. All the statistics are averaged based on 10 independent trails.

#### B. Greedy criteria in OGL

In this section, we examine the role of the greedy criterion in OGL via comparing the performance of OGL1, OGL2, OGL3 and OGLR. Let  $m_1=1000,\ m_2=1000$  and n=300 throughout this subsection. Fig. 3 shows the performance of OGL with four different greedy criteria. We observe that OGL1, OGL2 and OGL3 have similar performance, while OGLR performs worse. This shows that SGD is not the unique greedy criterion and shows the necessity to study the "greedy criterion" issue. Detailed comparisons are listed in the Table I. Here TestRMSE and  $k_{OGL}^*$  denote the theoretically optimal RMSE and number of iteration, where the parameter k is selected according to the test data directly.

TABLE I: Quantitive comparisons of OGL with different greedy criteria.

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Methods	TestRMSE	$k_{OGL}^*$	Methods	TestRMSE	$k_{OGL}^*$
$\sigma = 0.1$			$\sigma = 0.5$		
OGL1	0.0249	9	OGL1	0.0448	7
OGL2	0.0248	9	OGL2	0.0436	8
OGL3	0.0251	10	OGL3	0.0466	8
OGLR	0.0304	9	OGLR	0.0647	9
Methods	TestRMSE	$k_{OGL}^*$	Methods	TestRMSE	$k_{OGL}^*$
$\sigma = 1$			$\sigma = 2$		
OGL1	0.0780	7	OGL1	0.1371	5
OGL2	0.0762	7	OGL2	0.1374	7
OGL3	0.0757	7	OGL3	0.1377	7
OGLR	0.0995	7	OGLR	0.1545	6

## C. Feasibility of " $\delta$ -greedy threshold"

In this simulation, we aim at verifying the feasibility of the " $\delta$ -greedy threshold" criterion. For this purpose, we select optimal k according to the test data directly and compare different greedy criteria satisfying Eq. (III.7). Fig. 4 shows the simulation results.

Different from the previous simulation, we find in this experiment that the optimal RMSE of TOGLR is similar as that of TOGL1, TOGL2 and TOGL3. The main reason is that TOGL appends atom satisfying the " $\delta$ -greedy threshold" criterion Eq. (III.7). It implies that once an appropriately value of  $\delta$  is preset, then the selection of the atom is not relevant. Therefore, it agrees with Theorem III.1 and demonstrates that the introduced " $\delta$ -greedy threshold" is feasible. We also present quantitive comparisons in the Table II.

In Table II, the second column (" $\delta$  and k") compares the optimal  $\delta$  and corresponding k (in the bracket) derived only from Eq. (III.8) in TOGL. We also use  $k_{TOGL}^*$  to denote the optimal k (with the best performance). The aim of recording these quantities is to verify that only using Eq. (III.8) to build up the terminate criterion is not sufficient. In fact, TABLE II shows that for some data distributions, Eq. (III.8) fails to find out the optimal number of iteration k. Compared Table II with Table I, we find the TestRMSE derived from TOGL is comparable with OGL, which states the feasibility of TOGL.

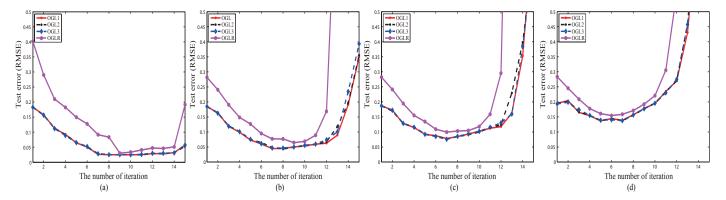


Fig. 3: The generalization performance of OGL with four different greedy criteria. (a) The noise level  $\sigma_1 = 0.1$ . (b)  $\sigma_2 = 0.5$ . (c)  $\sigma_3 = 1$ . (d)  $\sigma_4 = 2$ .

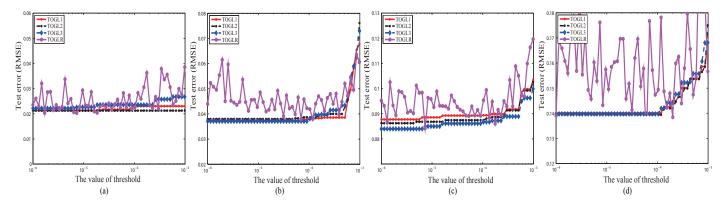


Fig. 4: The generalization performance of TOGL with four different greedy criteria. (a) The noise level  $\sigma_1 = 0.1$ . (b)  $\sigma_2 = 0.5$ . (c)  $\sigma_3 = 1$ . (d)  $\sigma_4 = 2$ .

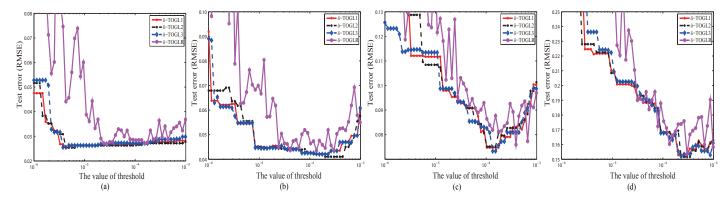


Fig. 5: The generalization performance of  $\delta$ -TOGL with four different greedy criteria. (a) The noise level  $\sigma_1 = 0.1$ . (b)  $\sigma_2 = 0.5$ . (c)  $\sigma_3 = 1$ . (d)  $\sigma_4 = 2$ .

## D. Feasibility of $\delta$ -TOGL

The only difference between  $\delta$ -TOGL and TOGL lies in the termination rule. Firstly we conduct the simulations to verify the feasibility of the termination rule Eq. (IV.2) in the Table III. Here, the second column ( $\delta$  and k) records the optimal  $\delta$  and corresponding k derived from the terminate rule Eq. (IV.2) in  $\delta$ -TOGL.  $k_{\delta-TOGL}^*$  denotes the optimal k selected according to the test samples. We see that the value of k obtained by Eq. (IV.2) is almost the same as  $k_{\delta-TOGL}^*$  for all four types of noise data. Furthermore, comparing Table III with TABLE

II, we find their TestRMSE are comparable. All these verify the feasibility and necessity of the termination rule Eq. (IV.2) in  $\delta$ -TOGL.

From OGL to  $\delta$ -TOGL, the main parameter changes from k to  $\delta$ . The following simulations aim at highlighting the role of the main parameters to illustrate the feasibility of  $\delta$ -TOGL. Similar to Fig. 3, we consider the relation between TestRMSE and the main parameter of  $\delta$ -TOGL in the Fig. 5. It can be found from Fig. 5 that although there may be additional oscillation within a small scope, the generalization capability

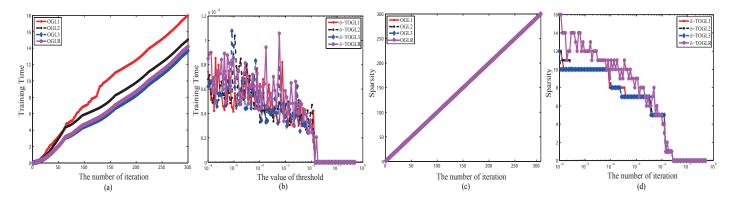


Fig. 6: The influence with respect to corresponding parameter changes on the training cost and sparsity in OGL and  $\delta$ -TOGL, respectively. (a) The training time of OGL. (b) The training time of  $\delta$ -TOGL. (c) The sparsity of the estimator in  $\delta$ -TOGL.

TABLE II: Quantitive comparisons for different greedy criteria

in TOGL

n TOGL.						
Methods	$\delta$ and $k$	TestRMSE	$k_{TOGL}^*$			
$\sigma = 0.1$						
TOGL1	[1.00e-6,3.58e-5]([9,13])	0.0213	8			
TOGL2	[1.00e-6,1.70e-6]([11,12])	0.0213	8			
TOGL3	[1.00e-6,1.70e-6]([12,13])	0.0222	10			
TOGLR	9.52e-6(12)	0.0203	11			
	$\sigma = 0.5$					
TOGL1	[1.00e-6,6.95e-5]([8,13])	0.0384	8			
TOGL2	[1.00e-6,4.67e-5]([9,13])	0.0390	8			
TOGL3	[1.00e-6,9.06e-5]([8,13])	0.0371	8			
TOGLR	6.95e-5(9)	0.0379	8			
$\sigma = 1$						
TOGL1	[1.00e-6,5.60e-6]([11,13])	0.0877	8			
TOGL2	[1.00e-6,4.30e-6]([11,13])	0.0862	8			
TOGL3	[1.00e-6,6.40e-6]([11,13])	0.0840	8			
TOGLR	7.30e-6(12)	0.0842	8			
$\sigma = 2$						
TOGL1	[1.00e-6,1.18e-4]([8,13])	0.1402	6			
TOGL2	[1.00e-6,1.18e-4]([8,13])	0.1404	6			
TOGL3	[1.00e-6,1.03e-4]([8,13])	0.1408	6			
TOGLR	6.09e-5(10)	0.1392	5			

of  $\delta$ -TOGL is not very sensitive to  $\delta$  on the whole, which is different from OGL (see Fig. 3).

We also examine the relation between training and test cost and the main parameter in OGL and  $\delta\text{-TOGL}$  to illustrate the feasibility of  $\delta\text{-TOGL}$ . As the test time mainly depends on the sparsity of the estimator, we record the sparsity instead. In this simulation, the scope of iterations in OGL starts from 0 to the size of dictionary (i.e., n=300) and our theoretical assertions reveal that the range of  $\delta$  in  $\delta\text{-TOGL}$  is (0,0.5]. We create 50 candidate values of  $\delta$  within  $[10^{-6},1/2]$ . It can be observed from the results in Fig. 6 that the training time (in seconds) and sparsity of  $\delta\text{-TOGL}$  is far less than OGL, which implies the computational amount of  $\delta\text{-TOGL}$  is much smaller than

TABLE III: Feasibility of the termination rule.

TABLE III. Feasibility of the termination rule.					
Methods	$\delta$ and $k$	TestRMSE	$k_{\delta-TOGL}^*$		
$\sigma = 0.1$					
δ-TOGL1	[4.30e-6,4.91e-6](11)	0.0255	11		
δ-TOGL2	[5.60e-6,6.40e-6]([10,11])	0.0254	10		
δ-TOGL3	3.76e-6(11)	0.0255	11		
$\delta$ -TOGLR	2.75e-5(11)	0.0268	11		
$\sigma = 0.5$					
δ-TOGL1	[1.18e-4,1.35e-4]([7,8])	0.0407	7		
δ-TOGL2	[2.01e-4,4.45e-4](7)	0.0401	7		
δ-TOGL3	[1.54e-4.2.29e-4]([7,8])	0.0407	7		
$\delta$ -TOGLR	1.35e-4([8,9])	0.0406	9		
$\sigma = 1$					
δ-TOGL1	[1.03e-4,1.76e-4]([7,8])	0.0747	7		
δ-TOGL2	[1.03e-4,1.54e-4]([7,8])	0.0752	7		
δ-TOGL3	[1.35e-4,1.54e-4]([7,8])	0.0733	7		
$\delta$ -TOGLR	3.89e-4([7,8])	0.0759	7		
$\sigma = 2$					
δ-TOGL1	[2.01e-4,2.99e-4]([6,7])	0.1529	6		
δ-TOGL2	[2.29e-4,3.41e-4]([6,7])	0.1516	6		
δ-TOGL3	2.29e-4([6,7])	0.1519	5		
$\delta$ -TOGLR	2.99e-4([7,8])	0.1537	6		
	•				

OGL.

## E. Comparisons

In this part, we compare  $\delta$ -TOGL with other classical dictionary-based learning schemes such as the pure greedy learning PGL [21], OGL [2], ridge regression [22] and Lasso [44]. We employ the  $\mathcal{L}_2$  regularized least-square (RLS) solution in ridge regression and the fast iterative shrinkage-thresholding algorithm (FISTA) in Lasso [4]. All the parameters, i.e., the number of iterations k in PGL or OGL, the regularization parameter  $\lambda$  in RLS or FISTA and the greedy threshold  $\delta$  in  $\delta$ -TOGL are all selected according to test dataset (or test RMSE) directly, since we mainly focus on the impact of the theoretically optimal parameter rather than validation techniques. The results are listed in Table IV, where the standard errors of test RMSE are also reported (numbers in

parentheses). From the results of Table IV, we observe that the

TABLE IV: Comparing the performance of  $\delta$ -TOGL with other classic algorithms.

lassic argorithms.						
Methods	Parameter	TestRMSE	Sparsity	Running time		
Regression function $sinc$ , dictionary $\mathcal{D}_n$ , $n = 300$ , noise level $\sigma = 0.1$						
PGL	k = 78	0.0284(0.0037)	78.0	27.4		
OGL	k = 9	0.0218(0.0034)	9.0	11.3		
δ-TOGL1	$\delta = 1.00e - 4$	0.0200(0.0044)	7.4	4.0		
δ-TOGL2	$\delta = 2.00e - 4$	0.0203(0.0064)	8.0	3.9		
δ-TOGL3	$\delta = 1.30e - 6$	0.0284(0.0074)	12.2	4.3		
δ-TOGLR	$\delta = 5.11e - 4$	0.0219(0.0059)	9.1	3.5		
$\mathcal{L}_2(RLS)$	$\lambda = 5e-5$	0.0313(0.0088)	300.0	0.5		
$\mathcal{L}_1(\text{FISTA})$	$\lambda = 5e-6$	0.0318(0.0102)	281.2	41.7		
Regression	function sinc, dict	ionary $\mathcal{D}_n, n = 10$	000, noise l	evel $\sigma = 0.1$		
PGL	k = 181	0.0278(0.0044)	181.0	116.6		
OGL	k = 9	0.0255(0.0045)	9.0	62		
δ-TOGL1	$\delta = 1.00e - 4$	0.0277(0.0072)	7.2	5.8		
δ-TOGL2	$\delta = 6.00e - 4$	0.0294(0.0119)	7.0	5.8		
δ-TOGL3	$\delta = 6.00e - 6$	0.0211(0.0036)	7.8	6.0		
δ-TOGLR	$\delta = 3.68e - 4$	0.0284(0.0082)	10.4	4.7		
$\mathcal{L}_2(RLS)$	$\lambda = 0.0037$	0.0322(0.0103)	1000.0	6.1		
$\mathcal{L}_1(\text{FISTA})$	$\lambda = 8e-6$	0.0317(0.0079)	821.2	103.7		
Regression	function sinc, dict	ionary $\mathcal{D}_n, n = 20$	000, noise le	evel $\sigma = 0.1$		
PGL	k = 263	0.0267(0.0036)	263.0	236.4		
OGL	k = 9	0.0250(0.0054)	9.0	374.7		
δ-TOGL1	$\delta = 2.00e - 4$	0.0256(0.0078)	7.1	9.5		
δ-TOGL2	$\delta = 1.00e - 4$	0.0280(0.0089)	8.6	9.3		
δ-TOGL3	$\delta = 2.00e - 6$	0.0222(0.0082)	7.6	9.2		
δ-TOGLR	$\delta = 4.176e - 5$	0.0266(0.0079)	10.6	6.7		
$\mathcal{L}_2(RLS)$	$\lambda = 0.0005$	0.0305(0.0088)	2000.0	28.9		
$\mathcal{L}_1(\text{FISTA})$	$\lambda = 7e-6$	0.0335(0.0079)	1252.4	176.3		

sparsities (or the number of selected atoms) of greedy-type strategies are far smaller than regularization-based methods, while they enjoy better performance. It empirically verifies that greedy-type algorithms are more suitable for redundant dictionary learning, which is also consistent with [2].

Furthermore, it can be found in Table IV that, although the generalization performance of all the aforementioned learning schemes are similar,  $\delta$ -TOGL finishes the corresponding learning task within a remarkably short period of running time. Although PGL has a lower computation complexity than OGL, its convergence rate is quite slow. Generally, PGL needs tens of thousands of iterations to guarantee performance, just as we preset the maximun of the default number of iteration of PGL is 10000 in the numerical studies. Therefore the applicable range of PGL is restricted. OGL possesses almost optimal convergence rate and generally converges within a few number of iterations. However, its computation complexity is huge, especially in large-scale dictionary learning. Table IV shows that, when the size of dictionary n are 300 and 1000, OGL performs faster than PGL, however it is much slower than PGL when n is 2000.

 $\delta$ -TOGL can significantly reduce the computation cost of OGL without sacrificing its generalization performance and sparsity, just as the results of  $\delta$ -TOGL1,  $\delta$ -TOGL2,  $\delta$ -TOGL3

and  $\delta$ -TOGLR shown in Table IV. It is mainly due to an appropriate " $\delta$ -greedy threshold" effective filtering a mass of "dead atoms" from the dictionary. We also notice that,  $\delta$ -TOGLR not only owns the good performance but also has the lowest computation complexity among the four  $\delta$ -TOGL learning schemes. It implies that, selecting the "active atom" from the dictionary without traversal can further reduce the complexity without deteriorating the performance of OGL.

#### VI. REAL DATA EXPERIMENTS

We have verified that  $\delta$ -TOGL is a feasible learning scheme in previous simulations. Especially,  $\delta$ -TOGLR possesses both good generalization performance and the lowest computation complexity. We now verify the learning performance of  $\delta$ -TOGLR on five real data sets and compare it with other classical dictionary-based learning methods including PGL, OGL, RLS and FISTA.

The first dataset is the Prostate cancer dataset [5]. The data set consists of the medical records of 97 patients who have received a radical prostatectomy. The predictors are 8 clinical measures and 1 response variable. The second dataset is the Diabetes data set [20]. This data set contains 442 diabetes patients that are measured on 10 independent variables and 1 response variable. The third one is the Boston Housing data set created form a housing values survey in suburbs of Boston by Harrison [25]. The Boston Housing dataset contains 506 instances which include 13 attributions and 1 response variable. The fourth one is the Concrete Compressive Strength (CCS) dataset [50], which contains 1030 instances including 8 quantitative independent variables and 1 dependent variable. The fifth one is the Abalone dataset[33] collected for predicting the age of abalone from physical measurements. The data set contains 4177 instances which were measured on 8 independent variables and 1 response variable.

Similarly, we randomly divide all the real data sets into two disjoint equal parts. The first half serves as the training set and the second half serves as the test set. We also use the Z-score standardization method [27] to normalize the data sets, in order to avoid the error caused by considerable magnitude difference among data dimensions. For each real data experiment, Gaussian radial basis function is also used to build up the dictionary:

$$\left\{ e^{-\|x-t_i\|^2/\eta^2} : i = 1, \dots, n \right\},\,$$

where  $\{t_i\}_{i=1}^n$  are drawn as the training samples themselves, thus the size of dictionary equals to training samples. We set the standard deviation of radial basis function as  $\eta = \frac{d_{max}}{\sqrt{2n}}$ , where  $d_{max}$  is maximum distance among all centers  $\{t_i\}_{i=1}^n$ , in order to avoid the radial basis function is too sharp or flat.

Table V documents the experimental results of generalization performance and running time on aforementioned five real data sets. We can clearly observe that, for the small-scale dictionary, i.e., for the Prostate data set, although  $\delta$ -TOGLR can achieve good performance, its running cost is greater than OGL and RLS. In fact, for each candidate threshold parameter  $\delta$ , a different iteration of the algorithm is needed run from scratch, which cancels the computational advantage

of  $\delta$ -TOGLR in small size dictionary learning. However, we also notice that, for the middle-scale dictionary, i.e., Diabetes, Housing and CCS,  $\delta$ -TOGLR begin to gradually surpass the other learning methods in computation with maintaining similar generalization performance as OGL. Especially for the large-scale dictionary learning, i.e., Abalone,  $\delta$ -TOGLR dominates other methods with a large margin in computation complexity and still possesses good performance.

#### VII. CONCLUSION AND FURTHER DISCUSSIONS

In this paper, we study the greedy criteria in orthogonal greedy learning (OGL). The main contributions can be concluded in four aspects.

Firstly, we propose that the steepest gradient descent (SGD) is not the unique greedy criterion to select atoms from dictionary in OGL, which paves a new way for exploring greedy criterion in greedy learning. To the best of our knowledge, this may be the first work concerning the "greedy criterion" issue in the field of supervised learning. Secondly, motivated by a series of previous researches of Temlyakov and his co-authors in greedy approximation [38], [40], [41], [42], [31], we eventually use the " $\delta$ -greedy threshold" criterion to quantify the level of greed for the learning purpose. Our theoretical result shows that OGL with such a greedy criterion yields a learning rate as  $m^{-1/2}(\log m)^2$ , which is almost the same as that of the classical SGD-based OGL in [2]. Thirdly, based on the " $\delta$ -greedy threshold" criterion, we derive an adaptive terminal rule for the corresponding OGL and thus provide a complete new learning scheme called as  $\delta$ thresholding orthogonal greedy learning ( $\delta$ -TOGL). We also present the theoretical demonstration that  $\delta$ -TOGL can reach the existing (almost) optimal learning rate just as the iterationbased termination rule dose in [2]. Finally, we analyze the generalization performance of  $\delta$ -TOGL and compare it with other popular dictionary-based learning methods including pure greedy learning PGL, OGL, ridge regression and Lasso through plenty of numerical experiments. The empirical results verify that the  $\delta$ -TOGL is a promising learning scheme, which possesses the good generalization performance and learns much faster than conventional methods in large-scale dictionary.

# APPENDIX A PROOFS

Since Theorem III.1 can be derived from Theorem IV.1 directly, we only prove Theorem IV.1 in this section. The methodology of proof is somewhat standard in learning theory. In fact, we use the error decomposition strategy in [29] to divide the generalization error into approximation error, sample error and hypothesis error. The main difficult of the proof is to bound the hypothesis error. The main tool to bound it is borrowed from [42].

In order to give an error decomposition strategy for  $\mathcal{E}(f_{\mathbf{z}}^k) - \mathcal{E}(f_{\rho})$ , we need to construct a function  $f_k^* \in \operatorname{span}(D_n)$  as follows. Since  $f_{\rho} \in \mathcal{L}_{1,\mathcal{D}_n}^r$ , there exists a  $h_{\rho} := \sum_{i=1}^n a_i g_i \in \operatorname{Span}(\mathcal{D}_n)$  such that

$$||h_{\rho}||_{\mathcal{L}_{1,\mathcal{D}_{n}}} \le \mathcal{B}, \text{ and } ||f_{\rho} - h_{\rho}|| \le \mathcal{B}n^{-r}.$$
 (A.1)

Define

$$f_0^* = 0, \ f_k^* = \left(1 - \frac{1}{k}\right) f_{k-1}^* + \frac{\sum_{i=1}^n |a_i| \|g_i\|_{\rho}}{k} g_k^*, \ \ (A.2)$$

where

$$g_k^* := \arg\max_{g \in \mathcal{D}_n'} \left\langle h_\rho - \left(1 - \frac{1}{k}\right) f_{k-1}^*, g \right\rangle_\rho,$$

and

$$\mathcal{D}'_n := \{g_i(x) / \|g_i\|_\rho\}_{i=1}^n \left\{ \left. \int \{-g_i(x) / \|g_i\|_\rho\}_{i=1}^n \right\} \right\}$$

with  $g_i \in \mathcal{D}_n$ .

Let  $f_{\mathbf{z}}^{\delta}$  and  $f_{k}^{*}$  be defined as in Algorithm 1 and Eq. (A.2), respectively, then we have

$$\mathcal{E}(\pi_{M} f_{\mathbf{z}}^{\delta}) - \mathcal{E}(f_{\rho})$$

$$\leq \mathcal{E}(f_{k}^{*}) - \mathcal{E}(f_{\rho}) + \mathcal{E}_{\mathbf{z}}(\pi_{M} f_{\mathbf{z}}^{\delta}) - \mathcal{E}_{\mathbf{z}}(f_{k}^{*})$$

$$+ \mathcal{E}_{\mathbf{z}}(f_{k}^{*}) - \mathcal{E}(f_{k}^{*}) + \mathcal{E}(\pi_{M} f_{\mathbf{z}}^{\delta}) - \mathcal{E}_{\mathbf{z}}(\pi_{M} f_{\mathbf{z}}^{\delta}),$$

where  $\mathcal{E}_{\mathbf{z}}(f) = \frac{1}{m} \sum_{i=1}^{m} (y_i - f(x_i))^2$ .

Upon making the short hand notations

$$\mathcal{D}(k) := \mathcal{E}(f_k^*) - \mathcal{E}(f_\rho),$$

$$\mathcal{S}(\mathbf{z}, k, \delta) := \mathcal{E}_{\mathbf{z}}(f_k^*) - \mathcal{E}(f_k^*) + \mathcal{E}(\pi_M f_{\mathbf{z}}^{\delta}) - \mathcal{E}_{\mathbf{z}}(\pi_M f_{\mathbf{z}}^{\delta}),$$

and

$$\mathcal{P}(\mathbf{z}, k, \delta) := \mathcal{E}_{\mathbf{z}}(\pi_M f_{\mathbf{z}}^{\delta}) - \mathcal{E}_{\mathbf{z}}(f_k^*)$$

respectively for the approximation error, the sample error and the hypothesis error, we have

$$\mathcal{E}(\pi_M f_{\mathbf{z}}^{\delta}) - \mathcal{E}(f_{\rho}) = \mathcal{D}(k) + \mathcal{S}(\mathbf{z}, k, \delta) + \mathcal{P}(\mathbf{z}, k, \delta). \quad (A.3)$$

At first, we give an upper bound estimate for  $\mathcal{D}(k)$ , which can be found in Proposition 1 of [29].

**Lemma A.1.** Let  $f_k^*$  be defined in Eq. (A.2). If  $f_\rho \in \mathcal{L}_{1,\mathcal{D}_n}^r$ , then

$$\mathcal{D}(k) \le \mathcal{B}^2 (k^{-1/2} + n^{-r})^2. \tag{A.4}$$

To bound the sample and hypothesis errors, we need the following Lemma A.2.

**Lemma A.2.** Let y(x) satisfy  $y(x_i) = y_i$ , and  $f_{\mathbf{z}}^{\delta}$  be defined in Algorithm 1. Then, there are at most

$$C\delta^{-2}\log\frac{1}{\delta}\tag{A.5}$$

atoms selected to build up the estimator  $f_{\mathbf{z}}^{\delta}$ . Furthermore, for any  $h \in Span\{D_n\}$ , we have

$$||y - f_{\mathbf{z}}^{\delta}||_{m}^{2} \le 2||y - h||_{m}^{2} + 2\delta^{2}||h||_{\mathcal{L}_{1}(\mathcal{D}_{n})}.$$
 (A.6)

*Proof.* (A.5) can be found in [42, Theorem 4.1]. Now we turn to prove (A.6). Our termination rule guarantees that either  $\max_{g \in \mathcal{D}_n} |\langle r_k, g \rangle_m| \leq \delta \|r_k\|_m$  or  $\|r_k\| \leq \delta \|y\|_m$ . In the latter case the required bound follows form

$$||y||_{m} \leq ||y - h||_{m} + ||h||_{m}$$

$$\leq \delta(||y - h||_{m} + ||h||_{m})$$

$$\leq \delta(||f - h||_{m} + ||h||_{\mathcal{L}_{1}(\mathcal{D}_{n})}).$$

TABLE V: The comparative results of performance and running time on five real data sets						
Datasets Methods	Prostate	Diabetes	Housing	CCS	Abalone	
Dictionary size	n = 50	n = 220	n = 255	n = 520	n = 2100	
	Average performance					
$\delta$ -TOGLR	0.4208 (0.0112)	55.1226 (1.0347)	4.045 (0.4256)	7.1279 (0.3294)	2.2460 (0.0915)	
PGL	0.4280 (0.0081)	56.3125 (2.0542)	4.0716 (0.2309)	11.2803 (0.0341)	2.5880 (0.0106)	
OGL	0.5170 (0.0119)	54.6518 (2.8700)	3.9447 (0.1139)	6.0128 (0.1203)	2.1725 (0.0088)	
RLS	0.4415 (0.0951)	57.3886 (1.5854)	3.9554 (0.3236)	9.8512 (0.2693)	2.2559 (0.0514)	
FISTA	0.6435 (0.0151)	61.7636 (2.5811)	5.1845 (0.1859)	12.8127 (0.3019)	3.4161 (0.0774)	
Average running time						
$\delta$ -TOGLR	0.58	1.11	0.89	0.82	4.22	
PGL	41.93	49.06	52.04	79.93	193.97	
OGL	0.16	1.11	1.42	7.46	787.2	
RLS	0.15	0.27	0.33	1.20	42.59	
FISTA	0.52	1.11	1.40	9.04	257.8	

TABLE V: The comparative results of performance and running time on five real data sets

Thus, we assume  $\max_{g \in \mathcal{D}_n} |\langle r_k, g \rangle_m| \le \delta ||r_k||_m$  holds. By using

$$\langle y - f_k, f_k \rangle_m = 0,$$

we have

$$||r_{k}||_{m}^{2} = \langle r_{k}, r_{k} \rangle_{m}$$

$$= \langle r_{k}, y - h \rangle_{m} + \langle r_{k}, h \rangle_{m}$$

$$\leq ||y - h||_{m} ||r_{k}||_{m} + \langle r_{k}, h \rangle_{m}$$

$$\leq ||y - h||_{m} ||r_{k}||_{m} + ||h||_{\mathcal{L}_{1}(\mathcal{D}_{n})} \max_{g \in \mathcal{D}_{n}} \langle r_{k}, g \rangle_{m}$$

$$\leq ||y - h||_{m} ||r_{k}||_{m} + ||h||_{\mathcal{L}_{1}(\mathcal{D}_{n})} \delta ||r_{k}||_{m}.$$

This finishes the proof.

Based on Lemma A.2 and the fact  $||f_k^*||_{\mathcal{L}_1(\mathcal{D}_n)} \leq \mathcal{B}$  [29, Lemma 1], we obtain

$$\mathcal{P}(\mathbf{z}, k, \delta) \le 2\mathcal{E}_{\mathbf{z}}(\pi_M f_{\mathbf{z}}^{\delta}) - \mathcal{E}_{\mathbf{z}}(f_k^*) \le 2\mathcal{B}\delta^2. \tag{A.7}$$

Now, we turn to bound the sample error  $\mathcal{S}(\mathbf{z},k)$ . Upon using the short hand notations

$$S_1(\mathbf{z}, k) := \{ \mathcal{E}_{\mathbf{z}}(f_k^*) - \mathcal{E}_{\mathbf{z}}(f_\varrho) \} - \{ \mathcal{E}(f_k^*) - \mathcal{E}(f_\varrho) \}$$

and

$$S_2(\mathbf{z}, \delta) := \{ \mathcal{E}(\pi_M f_{\mathbf{z}}^{\delta}) - \mathcal{E}(f_{\rho}) \} - \{ \mathcal{E}_{\mathbf{z}}(\pi_M f_{\mathbf{z}}^{\delta}) - \mathcal{E}_{\mathbf{z}}(f_{\rho}) \},$$

we write

$$S(\mathbf{z},k) = S_1(\mathbf{z},k) + S_2(\mathbf{z},\delta). \tag{A.8}$$

It can be found in Proposition 2 of [29] that for any 0 < t < 1, with confidence  $1 - \frac{t}{2}$ ,

$$S_1(\mathbf{z}, k) \le \frac{7(3M + \mathcal{B}\log\frac{2}{t})}{3m} + \frac{1}{2}\mathcal{D}(k)$$
 (A.9)

Using [49, Eqs(A.10)] with k replaced by  $C\delta^{-2}\log\frac{1}{\delta}$ , we have

$$S_2(\mathbf{z}, \delta) \le \frac{1}{2} \mathcal{E}(\pi_M f_{\mathbf{z}}^{\delta}) - \mathcal{E}(f_{\rho}) + \log \frac{2}{t} \frac{C\delta^{-2} \log \frac{1}{\delta} \log m}{m}$$
(A.10)

holds with confidence at least 1-t/2. Therefore, (A.3), (A.4), (A.7), (A.9), (A.10) and (A.8) yields that

$$\mathcal{E}(\pi_M f_{\mathbf{z}}^{\delta}) - \mathcal{E}(f_{\rho})$$

$$\leq C\mathcal{B}^2((m\delta^2)^{-1}\log m\log\frac{1}{\delta}\log\frac{2}{t} + \delta^2 + n^{-2r})$$

holds with confidence at least 1-t. This finishes the proof of Theorem IV.1.

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