Greedy metrics in orthogonal greedy learning ✤

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Abstract

Orthogonal greedy learning (OGL) is a stepwise learning scheme that adds a new atom from a dictionary via the steepest gradient descent and build the estimator via orthogonal projecting the target function to the space spanned by the selected atoms in each greedy step. Here, “greed” means choosing a new atom according to the steepest gradient descent principle. OGL then avoids the overfitting/underfitting by selecting an appropriate iteration number. In this paper, we point out that the overfitting/underfitting can also be avoided via redefining “greed” in OGL. To this end, we introduce a new greedy metric, called δ-greedy thresholds, to refine “greed” and theoretically verifies its feasibility. Furthermore, we reveals that such a greedy metric can bring an adaptive termination rule on the premise of maintaining the prominent learning performance of OGL. Our results show that the steepest gradient descent is not the unique greedy metric of OGL and some other more suitable metric may lessen the hassle of model-selection of OGL.

Keywords: Supervised learning, orthogonal greedy learning, greedy metric, thresholding, generalization capability.

1. Introduction

Supervised learning focuses on synthesizing a function (or mapping) to approximate (or represent) an underlying relationship between the input and corresponding output based on finitely many input-output samples. A system tackling supervised learning problems is

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commonly called as a learning system (or learning machine). A standard learning system usually comprises a hypothesis space, an optimization strategy, and a learning algorithm; Specifically, the hypothesis space is a family of parameterized functions that encodes the prior knowledge of the data, and the optimization strategy is an optimization problem which defines the estimator by utilizing the given samples, and the learning algorithm is an inference procedure that numerically solves the optimization problem.

Dictionary learning is a family of learning systems whose hypothesis spaces are linear combinations of atoms (or elements) of some given dictionaries. Here, the dictionary denotes a family of base learners \[32\]. For such type hypothesis spaces, regularization schemes such as the bridge estimator \[1\], ridge estimator \[18\] and Lasso estimator \[35\] are often employed as the optimization strategies. When the scale of samples is not too large, these optimization strategies can be realized by various learning algorithms such as the regularized least square algorithms \[39\], iterative thresholding algorithms \[12\] and iterative reweighted algorithms \[13\]. However, a large portion of the aforementioned learning algorithms are time-consuming and therefore may cause the sluggishness of the corresponding learning systems \[38\], particularly, when applied to the large-scale data sets.

Greedy learning or, more specifically, learning through greedy search or applying greedy-type algorithms, provides a possibility to circumvent the drawbacks of regularization methods \[2\]. Greedy-type algorithms are stepwise inference processes that start from a null model and follow the problem solving heuristic of making the locally optimal choice at each step with the hope of finding a global optimum. If the number of steps is moderate, then greedy-type algorithms possess charming computational advantage, when compared with the regularization schemes \[32\]. This property triggers avid research activities of greedy-type algorithms in signal processing \[11, 20, 36\], inverse problem \[16, 37\], sparse approximation \[15, 34\] and, particularly, machine learning \[2, 7, 21\].

1.1. Elements of greedy learning

Four most important elements of greedy learning are the “dictionary-selection”, “greedy-metric”, “iterative-strategy” and “stopping-criterion”. This is essentially different from
the greedy approximation that usually only focuses on the “dictionary-selection” and “iterative-format” issues [32], as the greedy learning concerns not only the approximation capability, but also the cost, such as the model complexity, that should pay to achieve a specified approximation accuracy. Therefore, greedy learning can be regarded as a four-issue learning scheme.

• “Dictionary-selection” issue: 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 [32], quasi-greedy basis [31], redundant dictionary [14], orthogonal basis [28], kernel-based sample dependent dictionary [6, 21] and stump dictionary [17].

• “Greedy-metric” issue: this issue regulates the criterion to choose a new atom (or element) from the dictionary in each greedy step. Besides the widely used steepest gradient descent (SGD) method [14], there are also many existing methods such as weak greed [29], thresholding greed [32] and super greed [23] to quantify the greedy-metric for the approximation purpose. However, to the best of our knowledge, only the SGD metric is employed in greedy learning, as all the results in [23, 29, 32] imply that this metric is superior to other metrics in greedy approximation.

• “Iterative-format” issue: this issue focuses on how to define a new estimator based on the selected atoms. Similar to the “dictionary-selection” issue, the “iterative-strategy” issue is also a classical topic of greedy approximation. There are several existing types of greedy iteration schemes [32]. Among these, three most commonly used iteration schemes are the pure greedy, orthogonal greedy and relaxed greedy formats. Each format possess its own pros and cons [31, 32] and has been widely used in greedy approximation and learning [2, 6, 17, 22, 33]. For instance, compared with the orthogonal greedy strategy, the pure and relaxed greedy strategies have benefits of computation but suffer from either the low convergence rate or the small applicable scope problem.

• “Stopping-criterion” issue: this issue depicts how to terminate the learning process. The “stopping-criterion” is regarded as the main distinction between greedy approximation and learning and has been frequently studied recently [2, 6, 21]. For example, Barron et al. [2] proposed an $l^0$-based complexity regularization strategy, and Chen et al. [6]
provided an $l^1$-based adaptive stopping criterion.

1.2. Motivations of greedy metrics

Orthogonal greedy learning (OGL) is a stepwise learning scheme that adds a new atom from a dictionary via SGD and then generate an estimator via orthogonally projecting the objective function to the space spanned by the selected atoms at each greedy step. A common consensus of orthogonal greedy approximation is that better approximation results can be achieved with larger number of iterations [32]. However, this claim cannot be applicable to greedy learning since the estimator is based on the samples with observational noises. Therefore, researches usually adopt a suitable number of iteration in OGL to avoid the overfitting/underfitting [2, 6].

![Figure 1: The comparisons among four OGL with different greedy metrics. The levels of greed satisfies OGL1 $\geq$ OGL2 $\geq$ OGL3 $\geq$ OGLR](image)

Since OGL always searches the most correlative atom and realizes the optimal approximation capability of the space spanned by the selected atoms in each greedy step, its generalization capability becomes sensitive to the number of iterations. Thus, a slight turbulence of the number of atoms may lead to a great change of the generalization capability, which can be witnessed in Fig.1. Furthermore, the $l^0$-based complexity regularization strategy [2] is only for the benefit of theoretical analysis and the applicable range of the $l^1$-based adaptive stopping criterion [6] is quite restricted, which makes it be difficult to persuade the programmers to utilize OGL. Recalling that a possible reason
of this problem is OGL searches the new atom according to SGD, an advisable idea is to weaken the level of greed by taking the “greedy-metric” issue into account. For this purpose, we run a simple simulation (whose experimental setting can be found in Sec. 5.2) to judge the possibility of this idea. The result (Fig.1) shows that the generalization of OGL will not degrade via weakening the level of greed if the greedy-metric is specified appropriately.

1.3. Our contributions

Different from other three issues of greedy learning, the “greedy metric” issue, to the best of our knowledge, has been studied a few in both theory and practice. The purpose of the present paper is to reveal the importance and necessity of studying the “greedy-metric” issue in OGL. The main contributions can be summarized as the following.

- We propose a new greedy metric called the “δ-greedy thresholds” to measure the level of greed in OGL. Although this metric has already been used in greedy approximation [32], the novelty of translating it to OGL is that using this metric in OGL provides a possibility to improve the generalization capability of OGL further. We prove that, if the iteration number is appropriately specified, then OGL with the “δ-greedy thresholds” metric can reach the existing almost optimal learning rate of OGL [2].

- Based on the “δ-greedy thresholds”, an adaptive termination rule is developed for OGL. Different from the classical stopping criterion that reach the bias and variance balance via choosing appropriate number of iterations, our study implies that the balance can also be attained through setting a suitable greedy metric. This phenomenon reveals the essential importance of the “greedy-metric” issue, which often seems to be overlooked in greedy learning. We also presents the theoretical justification of such an adaptive termination rule. Our result (Theorem 3.2) shows that the greedy-metric based termination rule performs as good as the iteration number based termination rule [2] in the sense that the generalization capabilities of the corresponding OGL are almost identical.

1.4. Organization

The rest of paper is organized as follows. In the next section, we make a brief introduction of statistical learning theory and greedy learning. In Section 3, we introduce the
“δ-greedy thresholds” metric in OGL and provide its feasibility justification. In Section 4, based on the “δ-greedy thresholds” metric, we propose an adaptive termination rule and the corresponding δ-TOGL system. The theoretical feasibility of the δ-TOGL system is also given in this section. In Section 5, we present numerical simulation experiments to verify our arguments. In Section 6, we provide the proofs of the main results. In the last section, we draw a simple conclusions of this paper.

2. Preliminaries

In this section, we present some preliminaries A fast review of the statistical learning theory as well as greedy learning is given in Sec.2.1 and Sec.2.2, respectively.

2.1. Statistical learning theory

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

\[
\rho(x, y) = \rho_X(x)\rho(y|x).
\]

Assume that \( f : X \to Y \) characterizes the correspondence between the input and output, as induced by \( \rho \). A natural measure of the error incurred by using \( f \) of this purpose is the generalization error, defined by

\[
\mathcal{E}(f) := \int_{Z} (f(x) - y)^2 d\rho,
\]

which is minimized by the regression function

\[
f_\rho(x) := \int_{Y} y d\rho(y|x).
\]

In general, since \( \rho \) is unknown, \( f_\rho \) is also unknown. However, we have access to random examples \( z \) from \( X \times Y \) sampled according to \( \rho \).

Let \( L_{\rho_X}^2 \) be the Hilbert space of \( \rho_X \) square integrable functions on \( X \), with norm \( \| \cdot \|_{\rho} \).

It is known that, for every \( f \in L_{\rho_X}^2 \), there holds

\[
\mathcal{E}(f) - \mathcal{E}(f_\rho) = \| f - f_\rho \|_{\rho}^2.
\]
So, the goal of learning is to find a best approximation of the regression function \( f_\rho \).

Let \( \mathcal{H} \) be a hypothesis space and \( f_\mathcal{H} \in \mathcal{H} \) be a best approximation of \( f_\rho \), i.e., \( f_\mathcal{H} = \arg \min_{g \in \mathcal{H}} \| g - f_\rho \|_\rho^2 \). Whenever there is an estimator \( f_\mathbf{z} \in \mathcal{H} \) based on the samples \( \mathbf{z} \) in hand, we have

\[
\mathcal{E}(f_\mathbf{z}) - \mathcal{E}(f_\rho) = \| f_\rho - f_\mathcal{H} \|_\rho^2 + \mathcal{E}(f_\mathcal{H}) - \mathcal{E}(f_\mathbf{z}).
\]

(2.2)

It is known [10] that a small \( \mathcal{H} \) will derive a large bias \( \| f_\rho - f_\mathcal{H} \|_\rho^2 \), while a large \( \mathcal{H} \) deduces a large variance \( \mathcal{E}(f_\mathcal{H}) - \mathcal{E}(f_\mathbf{z}) \). Thus the bias and variance are conflicting, and an ideal or best hypothesis space \( \mathcal{H}^* \) should be the one that best compromises the bias and the variance. This is the well known ”bias-variance” dilemma in statistical learning theory.

Without loss of generality, we always assume \( y \in [-M, M] \), and the number of samples is finite. Thus, it is reasonable to truncate the estimator to \([-M, M]\). That is, if we define

\[
\pi_M u = \begin{cases} 
  u, & \text{if } |u| \leq M \\
  M \text{sign}(u), & \text{otherwise}
\end{cases}
\]

as the truncation operator, then it is easy to deduce [42]

\[
\| \pi_M f_\mathbf{z} - f_\rho \|_\rho^2 \leq \| f_\mathbf{z} - f_\rho \|_\rho^2.
\]

2.2. Greedy learning

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

\[
\| f \|_{\mathcal{L}_1} := \inf_{\{a_g\}_{g \in D}} \left\{ \sum_{g \in D} |a_g| : f = \sum_{g \in D} a_g g \right\}.
\]

There exist several types of greedy algorithms [31]. Three most commonly used are the pure greedy (PGA), orthogonal greedy (OGA) and relaxed greedy (RGA) algorithms. In all the above greedy algorithms, we begin by setting \( f_0 := 0 \). The new approximation \( f_k (k \geq 1) \) is defined based on \( r_{k-1} := f - f_{k-1} \). In OGA, \( f_k \) is defined as

\[
f_k = P_{V_k} f,
\]
where $P_{V_k}$ is the orthogonal projection onto $V_k = \text{span}\{g_1, \ldots, g_k\}$ and $g_k$ is defined as
\[
g_k = \arg \max_{g \in D} |\langle r_{k-1}, g \rangle_H|.
\]

Given a set of training samples $z = (x_i, y_i)_{i=1}^m$, the empirical inner product and norm are defined by
\[
\langle f, g \rangle_m := \frac{1}{m} \sum_{i=1}^m f(x_i)g(x_i), \quad \|f\|_m := \frac{1}{m} \sum_{i=1}^m |f(x_i)|^2.
\]

The initial setting of OGL is the same as that of OGA. However, OGL should take the following four issues into account:

(I) **Dictionary-selection:** Select a dictionary $D_n := \{g_1, \ldots, g_n\}$ with $\|g_i\|_m \leq 1$.

(II) **Greedy-definition:**
\[
g_k = \arg \max_{g \in D_n} |\langle r_{k-1}, g \rangle_m|.
\]

(III) **Iteration-strategy:**
\[
f^k_z = P_{V^k_z} f,
\]
where $P_{V^k_z}$ is the orthogonal projection onto $V_k = \text{span}\{g_1, \ldots, g_k\}$ in the metric of $\| \cdot \|_m$.

(IV) **Stopping criterion:** Terminate the learning process when $k$ satisfies a certain assumption.

3. **Greedy-metric in OGL**

Given a real functional $V : \mathcal{H} \to \mathbb{R}$, the Fréchet derivative of $V$ at $f$, $V'_f : \mathcal{H} \to \mathbb{R}$, is the linear functional such that for $g \in \mathcal{H}$,
\[
\lim_{\|g\|_{\mathcal{H}} \to 0} \frac{|V(f + g) - V(f) - V'_f(g)|}{\|g\|_{\mathcal{H}}} = 0,
\]
and the gradient of $V$ as a map $\text{grad}V : \mathcal{H} \to \mathcal{H}$ is defined by
\[
\langle \text{grad}V(f), g \rangle_{\mathcal{H}} = V'_f(g), \text{ for all } g \in \mathcal{H}.
\]

The greedy-metric adopted in (II) is to find $g_k \in D_n$ such that
\[
\langle -\text{grad}(A_m)(f^k_z-1), g \rangle = \sup_{g \in D_n} \langle -\text{grad}(A_m)(f^k_z-1), g \rangle,
\]
where $A_m(f) = \sum_{i=1}^{m} |f(x_i)^2 - y_i|^2$. Therefore, the classical greedy-metric is based on the steepest gradient descent of $r_{k-1}$ with respect to the dictionary $\mathcal{D}_n$. By normalizing the residual $r_k$, $k = 0, 1, 2, \ldots, n$, (II) equals to search $g_k$ satisfying

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

Geometrically, it means to search a $g_k$ minimizing the angle $\theta_k$ between $r_{k-1}/\|r_{k-1}\|_m$ and $g_k$, which is depicted as the following Fig.2.

![Figure 2: Classical greedy-metric](image)

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

$$|\cos \theta_1| \leq |\cos \theta_2| \leq \cdots \leq |\cos \theta_k| \leq |\cos \theta_{k+1}| \leq \cdots \leq |\cos \theta_n|,$$

or

$$\frac{|\langle r_0, g_1 \rangle_m|}{\|r_0\|_m} \geq \cdots \geq \frac{|\langle r_{k-1}, g_k \rangle_m|}{\|r_{k-1}\|_m} \geq \cdots \geq \frac{|\langle r_{n-1}, g_n \rangle_m|}{\|r_{n-1}\|_m},$$

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 is a $\delta \in [|\cos \theta_k|, |\cos \theta_{k+1}|]$, which quantifies whether an atom should be utilized to construct the final estimator. To be detailed, if $|\cos \theta_k| \geq \delta$, then $g_k$ is regarded as an “active atom” and can be employed to build the estimator, otherwise, $g_k$ is a “dead one” which should be deported.

Based on the above observations, we are interested in selecting arbitrary “active atom”, $g_k$, in $\mathcal{D}_n$, that is

$$\frac{|\langle r_{k-1}, g_k \rangle_m|}{\|r_{k-1}\|_m} \geq \delta. \quad (3.1)$$
If there is no $g_k$ satisfying (3.1), then the algorithm terminates. We call the greedy metric (3.1) as the “$\delta$-greedy thresholds” metric. In practice, the number of “active atom” is usually not unique. Under this circumstance, we can choose arbitrary (just) one “active atom” at each greedy iteration. Once the “active atom” is selected, then the algorithm comes into the next greedy iteration and the “active atom” is redefined. Through such a greedy-metric, we can develop a new orthogonal greedy learning scheme, called thresholding orthogonal greedy learning (TOGL). Instead of (II) and (IV) in OGL, the corresponding parts of TOGL are described as follows

(II.1) **Greedy-definition:** Let $g_k$ be an arbitrary atom from $\mathcal{D}_n$ satisfying

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

(IV.1) **Stopping criterion:** Terminate the learning process either there is not atom satisfying (3.1) or $k$ satisfies a certain assumption.

Before giving the theoretical analysis of TOGL, we should highlight the difference between (II), (IV) and (II.1), (IV.1), respectively. Without considering the termination-rule, the classical greedy metric (II) satisfies (II.1) since (II) always selects the greediest atom in each greedy iteration. (II.1) 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 [10], 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 gradually flavor than OGL. Compared with (IV), (IV.1) provides another termination condition that if all the atoms, $g$, in $\mathcal{D}_n$ satisfy

$$\frac{|\langle r_{k-1}, g \rangle_m|}{\|r_{k-1}\|_m} < \delta,$$  

(3.2) then the algorithm terminates. Programmers have asked us frequently why there is the requirement of termination concerning $k$ besides (3.2), since their practical experience implies that the termination condition (3.2) is sufficient. We emphasize that the terminal condition concerning $k$ is necessary in TOGL, as the numerical simulations usually do not face the worst case. Indeed, using only the stopping condition (3.2) may drive the
algorithm to select all atoms from $D_n$. For example, if the target function $f$ is almost orthogonal to the space spanned by the dictionary and the atoms in the dictionary are almost linear dependent (See Fig.3), then the selected $\delta$ should be very small and such a small $\delta$ can not distinguish which is the “active atom”. Consequently, the corresponding learning scheme selects all the atoms of dictionary and therefore degrades the generalization capability of OGL.

![Figure 3: Flaw of the single stopping condition](image)

Now we present a theoretical assessment of TOGL. At first, we give a few notations and concepts, which will be used throughout the paper. Let $\mathcal{L}_1(D_n) := \{ f : f = \sum_{g \in D_n} a_g g \}$ endowed with the norm $\|f\|_{\mathcal{L}_1(D_n)} := \inf \left\{ \sum_{g \in D_n} |a_g| : f = \sum_{g \in D_n} a_g g \right\}$. For $r > 0$, the space $\mathcal{L}_1^r$ is defined to be the set of all functions $f$ such that, there exists $h \in \text{span}\{D_n\}$ such that

$$\|h\|_{\mathcal{L}_1(D_n)} \leq B, \text{ and } \|f - h\| \leq B n^{-r}, \quad (3.3)$$

where $\| \cdot \|$ denotes the uniform norm for the continuous function space $C(X)$. The infimum of all such $B$ defines a norm (for $f$ ) on $\mathcal{L}_1^r$. It follows from [2] that (3.3) defines a interpolation space and is a natural assumption for the regression function in greedy learning. Indeed, this assumption has already been adopted in [2, 21] to analyze the learning capability of greedy learning. The following Theorem 3.1 illustrate the performance of TOGL and consequently, reveals the feasibility of the greedy-metric (II.1).
Theorem 3.1. Let $0 < t < 1$, $0 < \delta \leq 1/2$, and $f_{z}^{k,\delta}$ be the estimator deduced by TOGL. If $f_{\rho} \in \mathcal{L}_{1}^{r}$, then there exits a $k^{*} \in \mathbb{N}$ such that

$$
E(\pi_{M}f_{z}^{k^{*},\delta}) - E(f_{\rho}) \leq CB^{2}((m\delta^{2})^{-1}\log m \log \frac{1}{\delta} \log \frac{2}{t} + \delta^{2} + n^{-2r})
$$

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., $n \geq \mathcal{O}(m^{\frac{1}{4}})$, then our result shows that the generalization error bound of $\pi_{M}f_{z}^{k^{*},\delta}$ is asymptotically $\mathcal{O}(m^{-1/2}(\log m)^{2})$. 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 of OGL within a certain extent is a feasible way to circumvent the model selection problem of OGL. It should also be pointed out that different from OGL [2], there are two parameters, $k$ and $\delta$, in TOGL. Therefore, Theorem 3.1 only presents a theoretical verification that introducing the “$\delta$-greedy thresholds” 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 (IV.1) is urgent. This is the scope of the following section, where an adaptive stopping criterion with respect to $\delta$ is presented.

4. $\delta$-thresholding orthogonal greedy learning

In TOGL, besides the greedy threshold parameter $\delta$, the stopping criterion should be also adjusted appropriately, which may dampen the users’ spirits to employ it. To circumvent this, in this section, we will develop an adaptive stopping criterion based on the “$\delta$-greedy thresholds” metric. With this, we can develop a practically user-friendly orthogonal greedy type learning system.

It has been pointed out in the previous section that the reason of employing the terminal condition concerning $k$ in (IV.1) is to circumvent the extreme case for a full running of TOGL. As the high impact atoms are all selected in such a setting, they then lead the relative value of the residual, $\|r_{k-1}\|_{m}/\|y(\cdot)\|_{m}$, to be small, where $y(\cdot)$ is a function satisfies $y(x_{i}) = y_{i}, i = 1, \ldots, m$. Therefore, a preferable terminal condition is to quantify this relative value. Noting that $\delta$ has already been utilized to terminate the
algorithm, we append another terminal condition as
\[ \|r_{k-1}\|_m \leq \delta \|y(\cdot)\|_m \] (4.1)

to replace the condition concerning \( k \) in (IV.1). Based to this, we obtain a novel applicable learning system by using the following (IV.2) to substitute (IV.1) in TOGL.

(IV.2) **Stopping criterion:** Terminate the learning process if either (4.1) holds or there is no atom satisfying (3.1).

**Algorithm 1 \( \delta \)-TOGL**

- **Step 1 (Initialization):** Given data \( z = (x_i, y_i)_{i=1}^m \), dictionary \( D_n \), the greedy thresholds \( \delta \), and \( f_0 = 0 \). Let \( k := 0 \).

- **Step 2 (\( \delta \)-greedy thresholds):** Let \( g_k \) be an arbitrary atom from \( D_n \) satisfying
\[ \frac{|\langle r_{k-1}, g_k \rangle_m|}{\|r_{k-1}\|_m} \geq \delta. \]

- **Step 3 (Orthogonal projection iteration):** Let \( V_{z,k} = \text{Span}\{g_1, \ldots, g_k\} \). Compute the approximation \( f_{\delta,k}^{z} \) as:
\[ f_{\delta,k}^{z} = P_{z,V_{z,k}}(y) \]

and the residual:
\[ r_k := y - f_{\delta,k}^{z}, \]

where \( P_{z,V_{z,k}} \) is the orthogonal projection onto space \( V_{z,k} \) in the metric of \( \langle \cdot, \cdot \rangle_m \).

- **Step 4 (Iteration):** If
\[ \max_{g \in D_n} |\langle r_k, g \rangle_m| \leq \delta \|r_k\|_m \text{ or } \|r_k\|_m \leq \delta \|f\|_m, \]

then the algorithm terminates, otherwise let \( k := k + 1 \), and we turn to Step 2.

**Output:** Since the stopping criterion depends only on \( \delta \), we can write the final estimator as \( f_{\delta}^{z} \).

For such a setting, we succeed in avoiding the cumbersome parameter \( k \) and derive a stopping-criterion based only on \( \delta \). That is, the main parameter \( k \) of OGL \([2]\) is replaced by the greedy thresholds \( \delta \). Eventually, by utilizing the “\( \delta \)-greedy thresholds” metric and
its corresponding adaptive terminal rule (IV.2), we design a new learning system called \(\delta\)-thresholding orthogonal greedy learning (\(\delta\)-TOGL) as in the Algorithm 1.

The following Theorem 4.1 shows that if \(\delta\) is appropriately tuned, then the \(\delta\)-TOGL estimator \(f^\delta_z\) can realize the almost optimal generalization capability of OGL and TOGL.

**Theorem 4.1.** Let \(0 < t < 1\), \(0 < \delta \leq 1/2\), and \(f^\delta_z\) be defined in Algorithm 1. If \(f_\rho \in \mathcal{L}_r\), then the inequality

\[
\mathcal{E}(\pi_M f^\delta_z) - \mathcal{E}(f_\rho) \leq CB^2((m\delta^2)^{-1}\log m \log \frac{1}{\delta} \log \frac{2}{t} + \delta^2 + n^{-2r})
\]

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

If we choose \(n \geq O(m^{1/4})\) and \(\delta = O(m^{-1/4})\), then the learning rate of (4.2) asymptotically equals to \(O(m^{-1/2}(\log m)^2)\), which is the same as that of Theorem 3.1. Therefore, Theorem 4.1 implies that using (4.1) to replace the terminal condition concerning \(k\) in (IV.1) is theoretically feasible. From the viewpoint of implementation, the stopping criterion (IV.2) is far more user-friendly than that of (IV.1), since (IV.2) omits the parameter \(k\) of (IV.1) without scarifying the generalization capability of TOGL.

The most highlight of Theorem 4.1 is that it provides a totally different way to circumvent the overfitting phenomenon of OGL. It is known that the stopping criterion is crucial for OGL, but designing an effective stopping criterion is a awkward problem. Barron et al. [2] suggested to select \(k\) that minimizes a \(l^0\) based complexity regularization strategy, which often needs a full running before the best parameter is selected. Chen et al. [6] proposed a stopping criterion also leads to a long iterative procedure in practice and sometimes does not work. In short, all the aforementioned study of stopping-criterion attempted to design a terminal rule by controlling the number of iterations directly. Since the generalization capability of OGL is sensitive to the number of iterations, these schemes sometimes fails to get satisfactory effects. The terminal rule employed in the present paper is based on the study of the “greedy-metric” issue of greedy learning. Theorem 4.1 shows that, besides controlling the number of iterations directly, setting a greedy threshold to redefine the greed can also conducts an effective stopping criterion. Theorem 4.1 implies that this new stopping criterion 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 metric slows down the changes of bias and variance.

5. Numerical Studies

In this section, we present several numerical simulations to reveal the pros and cons of $\delta$-TOGL. We divide the description into seven subsections. Except for the first one, each subsection depicts a topic concerning $\delta$-TOGL.

5.1. Experimental settings and purpose

Data and dictionary: The samples $z = \{(x_i, y_i)\}_{i=1}^{m_1}$ are generated as follows. $\{x_i\}_{i=1}^{m_1}$ are drawn independently and identically according to the uniform distribution on $[-\pi, \pi]$. $\{y_i\}_{i=1}^{m_1}$ satisfies $y_i = f_\rho(x_i) + \mathcal{N}(0, \sigma^2)$ with $\mathcal{N}(0, \sigma^2)$ being the white noise and

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

To comprehensively reveal the performances of OGL, TOGL and $\delta$-TOGL, we adopt four levels of noise, that is, $\sigma$ is set to $\sigma_1 = 0.1$, $\sigma_2 = 0.5$, $\sigma_3 = 1$ and $\sigma_4 = 2$. The learning performances of different algorithms were then tested by applying the resultant estimators to the test set $z_{test} = \{(x_i^{(t)}, y_i^{(t)})\}_{i=1}^{m_2}$, which was generated similarly to $z$ but with a promise that $y_i^{(t)}$s were always taken to be $y_i^{(t)} = f_\rho(x_i^{(t)})$.

In each simulation, we use Gaussian radial basis function 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 as the best packing points in $[-\pi, \pi]$. Since, the aim of the simulations is not to pursue the best width of Gaussian radial basis function, but to compare $\delta$-TOGL with other learning schemes on the same dictionary, we always set $\eta = 1$ throughout this section.

Methods: For OGL and $\delta$-TOGL, we apply the QR decomposition to solve the corresponding least squares problem and then obtain the estimators $[25]$. We use four metrics in (II) and (II.1) respectively to illustrate different levels of greed. Here, we use abbreviations OGL1, OGL2, OGL3, TOGL1, TOGL2, TOGL3, and $\delta$-TOGL1, $\delta$-TOGL2.
\( \delta \)-TOGL3 to denote OGL, TOGL and \( \delta \)-TOGL with (II), and (II.1) replaced by

\[
g_k := \arg \max_{g \in D_n} |\langle r_{k-1}, g \rangle_m|, \\
g_k := \arg \text{second} \max_{g \in D_n} |\langle r_{k-1}, g \rangle_m|, \\
\text{and} \\
g_k := \arg \text{third} \max_{g \in D_n} |\langle r_{k-1}, g \rangle_m|. 
\]

Here, \( \arg \text{second} \max_{g \in D_n} \) and \( \arg \text{third} \max_{g \in D_n} \) means selecting \( g_k \) such that the second and third largest values of \( |\langle r_{k-1}, g \rangle_m| \) are attained, respectively. Furthermore, we use OGLR, TOGLR and \( \delta \)-TOGLR to denote OGL, TOGL, and \( \delta \)-TOGL with (II) and (II.1) replaced by

\[ g_k \text{ randomly selected from } D_n, \]

and

\[ g_k \text{ randomly selected from } D_\delta \text{ with } D_\delta = \{ g_j : \langle g_j, r_{k-1} \rangle_m \geq \delta \| r_{k-1} \|_m \}. \]

We also compare our methods with two widely used learning schemes such as ridge regression [18] and Lasso [35]. We use the analytic solutions to ridge regression [18] and implementing the fast iterative soft thresholding algorithm (FISTA) [3] for Lasso to deduce the corresponding estimators.

**Aims of simulations** The aims of the simulations can be concluded into six aspects. In Sec.5.2, we demonstrate that SGD is not the unique metric to define greed in OGL. Indeed, our simulation shows that OGL2 and OGL3 possess almost the same generalization capabilities as that of OGL1. In Sec.5.3, we illustrate that “\( \delta \)-greedy thresholds” is a feasible greedy metric. In Sec.5.4, we aim to provide numerical verification of the good performance of \( \delta \)-TOGL. In Sec.5.5, we analyze how the parameter \( \delta \) affects the training time and the sparsity of the estimator. In Sec.5.6, we conduct a phase-transition diagram to illustrate the usability and limitations of \( \delta \)-TOGL. In Sec.5.7, we compare \( \delta \)-TOGL with other widely used dictionary-based learning schemes and then show the feasibility of \( \delta \)-TOGL.

**Environment:** All numerical studies are implemented by MATLAB R2013a on a Windows personal computer with Core(TM) i7-3770 3.40GHz CPUs and RAM 4.00GB, and the statistics are averaged based on 50 independent trails.
5.2. Greedy metric of OGL

In this part, we illustrate that SGD is not the unique metric for OGL. To this end, we conduct simulations for \( f_\rho \) with the aforementioned four types of noise. We sample \( m_1 = 1000 \) training samples and \( m_2 = 1000 \) testing samples. The number of centers is set to \( n = 300 \). Under this setting, we run 5 times of simulations and describe its average test errors, which is measured by the rooted mean square error (RMSE), as functions of the number of iterations, \( k \), of OGL1, OGL2, OGL3 and OGLR. Since the optimal \( k \) is small and the test RMSE is very large when \( k \) is large, we only record the figures with \( k \in [0, 15] \). The experimental results are shown in the following Fig.4.

![Graphs showing the generalization capabilities of OGL with different greedy metrics](image)

Fig.4 (a)-(d) shows the learning capabilities of OGL for \( f_\rho \) with different levels of noise from \( \delta_1 \) to \( \delta_4 \). It can be found that OGL1, OGL2 and OGL3 possess almost the same generalization capabilities, since both the smallest test RMSE and the optimal \( k \)
of them are almost the same. This implies that, at least for a certain learning task, SGD is not the unique metric for OGL. Furthermore, it can also be found in Fig.4 that OGLR performs worse than that of other learning schemes. This phenomenon shows that introducing a greedy metric is necessary. We also give a quantitive comparison of the learning performances of OGL1, OGL2, OGL3, and OGLR in the following Tab.1. Here TestRMSE\textsubscript{OGL} and \(k^*_{\text{OGL}}\) denote the theoretically optimal test RMSEs and \(k\) of OGL with different greedy metrics. Indeed, \(k^*_{\text{OGL}}\)'s are selected according to the test data directly.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|}
\hline
Methods & TestRMSE\textsubscript{OGL} & \(k^*_{\text{OGL}}\) \\
\hline
\hline
\(\sigma = 0.1\) & & \\
OGL1 & 0.0249 & 9 \\
OGL2 & 0.0248 & 9 \\
OGL3 & 0.0251 & 10 \\
OGLR & 0.0304 & 9 \\
\hline
\hline
\(\sigma = 0.5\) & & \\
OGL1 & 0.0448 & 7 \\
OGL2 & 0.0436 & 8 \\
OGL3 & 0.0466 & 8 \\
OGLR & 0.0647 & 9 \\
\hline
\hline
\(\sigma = 1\) & & \\
OGL1 & 0.0780 & 7 \\
OGL2 & 0.0762 & 7 \\
OGL3 & 0.0757 & 7 \\
OGLR & 0.0995 & 7 \\
\hline
\hline
\(\sigma = 2\) & & \\
OGL1 & 0.1371 & 5 \\
OGL2 & 0.1374 & 7 \\
OGL3 & 0.1377 & 7 \\
OGLR & 0.1545 & 6 \\
\hline
\end{tabular}
\caption{OGL numerical average results for 5 simulations.}
\end{table}

All the above simulations show that greed is necessary but not unique in OGL. This stimulates us to launch a study of the “greedy-metric” issue of OGL.

5.3. “\(\delta\)-greedy thresholds” metric

In this part, we verify the feasibility of the “\(\delta\)-greedy thresholds” metric proposed in Sec.3. The simulation setting of this subsection is the same as that of Sec.5.2. We also run 5 times of simulations and describe its test RMSE as functions of the threshold, \(\delta\), of TOGL1, TOGL2, TOGL3 and TOGLR, where we choose the optimal number of iterations based on the test set. There are 100 candidates of \(\delta\) which are equally logarithmically drawn from \([10^{-6}, 1/2]\). Since the optimal value of \(\delta\) lies in \([10^{-6}, 0.001]\), we only plot the range of \(\delta\) in \([10^{-6}, 0.001]\) to present more details of the simulations. The experimental results are reported in the following Fig.5.
Fig. 5 shows that, different from Fig. 4, the learning capability of TOGLR is similar as that of TOGL1, TOGL2 and TOGL3. The main reason is that we select the new atom (even for the random selected atom) in a greedy fashion by adding the “δ-greedy thresholds” metric in TOGL. This phenomenon implies that once an appropriately δ is preset, then how to choose the atom according to (II.1) is not crucial. Therefore, it numerically verifies Theorem 3.1 and demonstrates that the introduced “δ-greedy threshold” is feasible and appropriate to quantify the greedy metric. To facilitate the comparison, we also record the optimal generalization errors in Tab. 2.

In Tab. 2, the second column (i.e., “δ and k”) records the optimal δ value and their corresponding k values (in the bracket) derived from TOGL. We should highlight that these k are obtained by using the terminal condition (3.2) only. We also use $k^*_{TOGL}$ to denote the theoretically optimal k of TOGL, which is selected based on the test set. It
can be found in Tab.2 that when $\delta$ equals to 0.1 or 0.5, the corresponding $k$ is almost the same as $k^*_TOGL$, which means that using the terminal condition (3.2) is sufficient to select the optimal iteration number. However, if the noise is enlarged, that is, $\delta = 1$ or 2, then the terminal condition (3.2) usually fails to find out the optimal $k$ and another stopping condition need to be employed. This explains why we introduce a terminal condition concerning $k$ in (IV.1) and an adaptive terminal condition (4.1) in (IV.2). Compared with Tab.1, we can find from Tab.2 that the optimal test RMSEs ($TestRMSE_{TOGL}$ and $TestRMSE_{OGL}$) are comparable, which illustrates that the “$\delta$-greedy thresholds” metric is feasible. The new greedy metric then provides an alternative way to enrich the model-selection strategy without sacrificing the generalization capability of OGL.

Table 2: TOGL numerical average results for 5 simulations.

| Methods | $\delta$ and $k$ | $TestRMSE_{TOGL}$ | $k^*_TOGL$ |
|---------|------------------|--------------------|------------|
| $\sigma = 0.1$ |
| 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   | $[1.00e-6,6.95e-5]\{[8,13]\}$ | 0.0374             | 8          |
| TOGL2   | $[1.00e-6,4.67e-5]\{[9,13]\}$ | 0.0380             | 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   | $[1.00e-6,1.18e-4]\{[8,13]\}$ | 0.1394             | 6          |
| TOGL3   | $[1.00e-6,1.03e-4]\{[8,13]\}$ | 0.1398             | 6          |
| TOGLR   | $6.09e-5\{10\}$ | 0.1282             | 5          |
5.4. The generalization capability of $\delta$-TOGL

In this part, we justify the good performance of $\delta$-TOGL proposed in Sec.4. The detailed experimental setting is the same as that in Sec.5.3. Different from TOGL, $\delta$-TOGL provides an adaptive terminal rule and therefore, eliminates the parameter $k$ in TOGL. Similarly to Sec.5.3, we only plot the range of $\delta$ in $[10^{-6}, 0.001]$ to reveal more details of the simulations. The following Fig.6 reports the simulations results.

![Figure 6: The feasibility of the $\delta$-TOGL](image)

Fig.6 shows that $\delta$-TOGL maintains the feasibility of “$\delta$-greedy thresholds” metric after introduced the adaptive termination rule (IV.2). Therefore, it numerically verifies Theorem 4.1 and demonstrates that $\delta$-TOGL is feasible. We also show the generalization capability of $\delta$-TOGL in the following Tab.3.
Table 3: δ-TOGL numerical average results for 5 simulations.

| Methods | δ and k | TestRMSE_{δ-TOGL} | k^*_δ-TOGL |
|---------|---------|-------------------|-------------|
|         |         | TestRMSE_{δ-TOGL} |             |
|         |         | k^*_δ-TOGL         |             |
| δ-TOGL1 | [4.30e-6,4.91e-6](11) | 0.0255 | 10.6 |
| δ-TOGL2 | [5.60e-6,6.40e-6](10.4) | 0.0254 | 10.2 |
| δ-TOGL3 | 3.76e-6(11) | 0.0255 | 10.6 |
| δ-TOGLR | 2.75e-5(11) | 0.0268 | 10.8 |
|         |         | TestRMSE_{δ-TOGL} |             |
|         |         | k^*_δ-TOGL         |             |
| δ-TOGL1 | [1.18e-4,1.35e-4](7.4) | 0.0521 | 7.4 |
| δ-TOGL2 | [2.01e-4,4.45e-4](7) | 0.0511 | 7 |
| δ-TOGL3 | [1.54e-4,2.29e-4](7.2) | 0.0520 | 7.2 |
| δ-TOGLR | 1.35e-4(8.6) | 0.0536 | 8.6 |
|         |         | TestRMSE_{δ-TOGL} |             |
|         |         | k^*_δ-TOGL         |             |
| δ-TOGL1 | [1.03e-4,1.76e-4](7.2) | 0.0747 | 6.8 |
| δ-TOGL2 | [1.03e-4,1.54e-4](7.2) | 0.0752 | 6.8 |
| δ-TOGL3 | [1.35e-4,1.54e-4](7.2) | 0.0733 | 7 |
| δ-TOGLR | 3.89e-4(7.2) | 0.0759 | 6.4 |
|         |         | TestRMSE_{δ-TOGL} |             |
|         |         | k^*_δ-TOGL         |             |
| δ-TOGL1 | [2.01e-4,2.99e-4](6.2) | 0.1529 | 5.4 |
| δ-TOGL2 | [2.29e-4,3.41e-4](6.2) | 0.1516 | 5.6 |
| δ-TOGL3 | 2.29e-4(6.2) | 0.1519 | 4.8 |
| δ-TOGLR | 2.99e-4(7.2) | 0.1537 | 6.2 |

In Tab.3, the second column (i.e., “δ and k”) records the optimal δ and the corresponding k (in the bracket) derived from δ-TOGL, and $k^*_δ-TOGL$ denotes the theoretically optimal k of δ-TOGL. It can be found that for all types of noise, k is almost the same as $k^*_δ-TOGL$. This shows that the stopping condition concerning k in (IV.1) can be substituted with the terminal condition (4.1). Therefore, these experimental results demonstrate in some extent that we can avoid the “overfitting” by only taking the “greedy-metric” issue into account. This can be regarded as the main novelty of our paper. Furthermore, noting that the optimal test RMSEs ($TestRMSE_{δ-TOGL}$) are comparable with $TestRMSE_{TOGL}$, we can declare that δ-TOGL performs as well as TOGL, while δ-TOGL successfully omit the parameter concerning k in TOGL.
5.5. The cost of alternating parameter of $\delta$-TOGL

From OGL to $\delta$-TOGL, the main parameter is changed from $k$ to $\delta$. In the previous subsections, we pointed out that the generalization capability of such a change was not degraded. Furthermore, $\delta$-TOGL provides a more user-friendly parametric selection strategy. The purpose of this part is to discuss how the training time and testing time of $\delta$-TOGL vary with $\delta$. Since the testing time depends only on the sparsity of the final estimator, we use the number of iterations to replace the testing time in this simulation. In this simulation, we only take the level of noise as $\sigma = 0.1$ and the other experimental setting is the same as that of Sec.5.4. The simulation results are reported in the following Fig.7.

![Figure 7](image)

Figure 7: The parameter’s influences on training and testing prices in OGL and $\delta$-TOGL

From Fig.7, it shows that the training and testing costs are not expensive when the parameter $\delta$ tuning in the range $[10^{-6}, 0.5]$, where the sparsity no more than 16 and the
corresponding training time is no more than $1.2 \times 10^{-3}$ second. All these show that when the parameter, $k$, of OGL is transformed as $\delta$ in $\delta$-TOGL, both the training and test burdens are not added.

5.6. Usability and limitations of $\delta$-TOGL

In this simulation experiments, we use $\delta$-TOGL1 to learn the sinc function with sampling noise as $N(0, 0.1^2)$. The horizontal axis represents the number of training samples, and the vertical axis represents the associated target accuracies (which will be defined as follows). Therefore, every point in the coordinate system denotes a given learning task. If the test RMSE of $\delta$-TOGL with $\delta$ selecting by 5-fold cross-validation is less than the accuracy, we define that the learning task is successful and labeled 1, otherwise, the tasks fails and tag 0. We run 100 times of trials in each point. The color from blue to red denotes the values from 0 to 100. The result is shown in the following Fig.8.

![Figure 8: Usability and limitations of $\delta$-TOGL](image)

In the above Fig.8, the red areas represents that $\delta$-TOGL meets the demand of learning task and the blue area indicates failure. And we can immediately acquire an intuitive enlightenment from the above phase transition diagram: given a set of data and a target accuracy for a specific learning task, if you want to use $\delta$-TOGL to have a try, then such phase transition diagram can tell you, how many samples are approximately needed to ensure the accomplishment of your mission within a certain probability. From the above experimental result, the generalization error of $\delta$-TOGL performances steadily, gradually
inversely monotonous to the sample size, which fits our theoretical results in Theorem

Table 4: Compared δ-TOGL performance with other classic algorithms.

| Methods    | Parameter | TestRMSE(standard error) | Sparsity |
|------------|-----------|--------------------------|----------|
| OGL        | $k = 9$   | 0.0218(0.0034)           | 9        |
| δ-TOGL1    | $\delta = 1.00e - 4$ | 0.0200(0.0044)           | 7.42     |
| δ-TOGL2    | $\delta = 2.00e - 4$ | 0.0203(0.0064)           | 8        |
| δ-TOGL3    | $\delta = 1.30e - 6$ | 0.0284(0.0074)           | 12.2     |
| δ-TOGLR    | $\delta = 3.80e - 4$ | 0.0219(0.0059)           | 9        |
| $\mathcal{L}_2$(RLS) | $\lambda = 5e-5$ | 0.0263(0.0098)           | 300      |
| $\mathcal{L}_1$(FISTA) | $\lambda = 5e-6$ | 0.0298(0.0092)           | 290.4    |
| OGL        | $k = 9$   | 0.0255(0.0045)           | 9        |
| δ-TOGL1    | $\delta = 1.00e - 4$ | 0.0277(0.0072)           | 7.2      |
| δ-TOGL2    | $\delta = 6.00e - 4$ | 0.0294(0.0119)           | 7        |
| δ-TOGL3    | $\delta = 6.00e - 6$ | 0.0211(0.0036)           | 7.8      |
| δ-TOGLR    | $\delta = 1.00e - 4$ | 0.0284(0.0082)           | 10.4     |
| $\mathcal{L}_2$(RLS) | $\lambda = 0.0037$ | 0.0272(0.0103)           | 1000     |
| $\mathcal{L}_1$(FISTA) | $\lambda = 7e-6$ | 0.0277(0.0094)           | 931.8    |
| OGL        | $k = 9$   | 0.0250(0.0054)           | 9        |
| δ-TOGL1    | $\delta = 2.00e - 4$ | 0.0256(0.0078)           | 7.14     |
| δ-TOGL2    | $\delta = 1.00e - 4$ | 0.0280(0.0089)           | 8.6      |
| δ-TOGL3    | $\delta = 2.00e - 6$ | 0.0222(0.0082)           | 7.6      |
| δ-TOGLR    | $\delta = 9.06e - 5$ | 0.0266(0.0079)           | 10.6     |
| $\mathcal{L}_2$(RLS) | $\lambda = 0.0005$ | 0.0256(0.0126)           | 2000     |
| $\mathcal{L}_1$(FISTA) | $\lambda = 7e-6$ | 0.0235(0.0079)           | 1772     |
5.7. $\delta$-TOGL is competitive

In this part, we compare $\delta$-TOGL with some classical dictionary-based learning schemes such as the classical OGL, ridge and lasso estimators. The regularization parameters of both ridge and lasso estimators, the iteration number of OGL and the threshold, $\delta$, of $\delta$-TOGL are drawn by using 5-fold cross-validation. The regression is the sinc function with sampling noise as the standard Gaussian noise with the variance 0.1, i.e., $\mathcal{N}(0, 0.1^2)$. The simulation result can be seen in Tab.4.

From Tab.4, we can see that under the same order of generalization performance magnitude, the number of selected atoms of greedy-type strategy is far smaller than the regularization algorithms. This explains why greedy-type algorithms are more suitable for redundant dictionary learning [2]. Furthermore, it also can be found in Tab.4 that the generalization capability of all the aforementioned learning schemes are similar. At last, our simulation results shows that the size of dictionary doesn’t affect the learning performance of $\delta$-TOGL schemes very much, provided it attains the lowest requirement to finishes the learning task. All these reveals that $\delta$-OGL is a competitive learning scheme.

6. Proofs

Since Theorem 3.1 can be regarded as a special case of Theorem 4.1, we only prove Theorem 4.1 in this section. The methodology of proof is the same as that of [21], and the main tool is borrowed from [33].

In order to give an error decomposition strategy for $\mathcal{E}(f^k_\rho) - \mathcal{E}(f_\rho)$, we need to construct a function $f^*_k \in \text{span}(D_n)$ as follows. Since $f_\rho \in \mathcal{L}_1^r$, there exists a $h_\rho := \sum_{i=1}^n a_i g_i \in \text{Span}(D_n)$ such that
\begin{equation}
\|h_\rho\|_{\mathcal{L}_1} \leq B, \text{ and } \|f_\rho - h_\rho\| \leq Bn^{-r}.
\end{equation}

Define
\begin{equation}
f^*_0 = 0, \quad f^*_k = (1 - \frac{1}{k}) f^*_{k-1} + \frac{\sum_{i=1}^n |a_i| \|g_i\|_\rho g^*_k}{k},
\end{equation}
where
\begin{align*}
g^*_k := \arg\max_{g \in \mathcal{D}_n^r} \left\langle h_\rho - \left(1 - \frac{1}{k}\right) f^*_{k-1}, g \right\rangle_\rho,
\end{align*}
and
\begin{align*}
h_\rho := \sum_{i=1}^n a_i g_i \in \text{Span}(D_n).
\end{align*}
and 
\[ D'_n := \{ g_i(x)/\|g_i\|_{\rho} \}_{i=1}^n \cup \{-g_i(x)/\|g_i\|_{\rho} \}_{i=1}^n \]
with \( g_i \in D_n \).

Let \( f^\delta_z \) and \( f^*_k \) be defined as in Algorithm 1 and (6.2), respectively, then we have
\[
\mathcal{E}(\pi_M f^\delta_z) - \mathcal{E}(f_{\rho}) \\
\leq \mathcal{E}(f^*_k) - \mathcal{E}(f_{\rho}) + \mathcal{E}_z(\pi_M f^\delta_z) - \mathcal{E}_z(f^*_k) \\
+ \mathcal{E}_z(f^*_k) - \mathcal{E}(f^*_k) + \mathcal{E}(\pi_M f^\delta_z) - \mathcal{E}(f^*_k),
\]
where \( \mathcal{E}_z(f) = \frac{1}{m} \sum_{i=1}^m (y_i - f(x_i))^2 \).

Upon making the short hand notations
\[
\mathcal{D}(k) := \mathcal{E}(f^*_k) - \mathcal{E}(f_{\rho}), \\
\mathcal{S}(z, k, \delta) := \mathcal{E}_z(f^*_k) - \mathcal{E}(f^*_k) + \mathcal{E}(\pi_M f^\delta_z) - \mathcal{E}_z(f^*_k),
\]
and
\[
\mathcal{P}(z, k, \delta) := \mathcal{E}_z(\pi_M f^\delta_z) - \mathcal{E}_z(f^*_k)
\]
respectively for the approximation error, the sample error and the hypothesis error, we have
\[
\mathcal{E}(\pi_M f^\delta_z) - \mathcal{E}(f_{\rho}) = \mathcal{D}(k) + \mathcal{S}(z, k, \delta) + \mathcal{P}(z, k, \delta). \quad (6.3)
\]

At first, we give an upper bound estimate for \( \mathcal{D}(k) \), which can be found in Proposition 1 of [21].

**Lemma 6.1.** Let \( f^*_k \) be defined in (6.2). If \( f_{\rho} \in \mathcal{L}^r_1 \), then
\[
\mathcal{D}(k) \leq B^2(k^{-1/2} + n^{-r})^2. \quad (6.4)
\]

To bound the sample and hypothesis errors, we need the following Lemma 6.2

**Lemma 6.2.** Let \( y(x) \) satisfy \( y(x_i) = y_i \), and \( f^\delta_z \) be defined in Algorithm 1. Then, there are at most
\[
C\delta^{-2} \log \frac{1}{\delta} \quad (6.5)
\]
bases selected to build up the estimator \( f^\delta_z \). Furthermore, for any \( h \in \text{Span}\{D_n\} \), we have
\[
\|y - f^\delta_z\|_m^2 \leq 2\|y - h\|_m^2 + 2\delta^2\|h\|_{\mathcal{L}_1(D_n)}. \quad (6.6)
\]
Proof. (6.5) can be found in [33, Theorem 4.1]. Now we turn to prove (6.6). Our stopping criterion 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

\[
\|y\|_m \leq \|y - h\|_m + \|h\|_m \leq \delta(\|y - h\|_m + \|h\|_m) \leq \delta(\|f - h\|_m + \|h\|_{\mathcal{L}_1(\mathcal{D}_n)}).
\]

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

\[
\langle y - f_k, f_k \rangle_m = 0,
\]

we have

\[
\|r_k\|_m^2 = \langle r_k, r_k \rangle_m = \langle r_k, y - h \rangle_m + \langle r_k, h \rangle_m \leq \|y - h\|_m \|r_k\|_m + \|r_k\|_m
\]

\[
\leq \|y - h\|_m \|r_k\|_m + \|h\|_{\mathcal{L}_1(\mathcal{D}_n)} \max_{g \in \mathcal{D}_n} \langle r_k, g \rangle_m \leq \|y - h\|_m \|r_k\|_m + \|h\|_{\mathcal{L}_1(\mathcal{D}_n)} \delta \|r_k\|_m.
\]

This finishes the proof. ■

Based on Lemma 6.2 and the fact \( \|f_k^*\|_{\mathcal{L}_1(\mathcal{D}_n)} \leq B \) [21, Lemma 1], we obtain

\[
\mathcal{P}(\mathcal{z}, k, \delta) \leq 2 \mathcal{E}_z(\pi_M f_k^\delta) - \mathcal{E}_z(f_k^*) \leq 2B \delta^2.
\] (6.7)

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

\[
S_1(\mathcal{z}, k) := \{\mathcal{E}_z(f_k^*) - \mathcal{E}_z(f_\rho)\} - \{\mathcal{E}(f_k^*) - \mathcal{E}(f_\rho)\}
\]

and

\[
S_2(\mathcal{z}, \delta) := \{\mathcal{E}(\pi_M f_k^\delta) - \mathcal{E}(f_\rho)\} - \{\mathcal{E}_z(\pi_M f_k^\delta) - \mathcal{E}_z(f_\rho)\},
\]

we write

\[
\mathcal{S}(\mathcal{z}, k) = S_1(\mathcal{z}, k) + S_2(\mathcal{z}, \delta).
\] (6.8)

It can be found in Proposition 2 of [21] that for any \( 0 < t < 1 \), with confidence \( 1 - \frac{t}{2} \),

\[
S_1(\mathcal{z}, k) \leq \frac{7(3M + B \log \frac{2}{\delta})}{3m} + \frac{1}{2} \mathcal{D}(k)
\] (6.9)

Using [41, Eqs(A.10)] with \( k \) replaced by \( C \delta^{-2} \log \frac{1}{\delta} \), we have

\[
S_2(\mathcal{z}, \delta) \leq \frac{1}{2} \mathcal{E}(\pi_M f_k^\delta) - \mathcal{E}(f_\rho) + \log \frac{2 C \delta^{-2} \log \frac{1}{\delta} \log m}{m}
\] (6.10)

holds with confidence at least \( 1 - t/2 \). Therefore, (6.3), (6.4), (6.7), (6.9), (6.10) and (6.8) yields that

\[
\mathcal{E}(\pi_M f_k^\delta) - \mathcal{E}(f_\rho) \leq CB^2((m \delta^2)^{-1} \log m \log \frac{1}{\delta} \log \frac{2}{t} + \delta^2 + n^{-2r})
\]

holds with confidence at least \( 1 - t \). This finishes the proof of Theorem 4.1.
7. Concluding Remarks

The main contributions of the present paper can be concluded into four folds. Firstly, we propose that the steepest gradient descent (SGD) is not the unique choice to select a new atom from dictionary in orthogonal greedy algorithm (OGL), which disrupts habitual thinking to make a way for searching new greedy metric for OGL. To the best of our knowledge, this is the first work on the “greedy-metric” issue for greedy learning. Secondly, we succeed in finding an appropriate greedy metric in OGL and theoretically and numerically verify its rationality and feasibility. Motivated by a series work of Temlyakov and his co-authors \[23, 29, 31, 32, 33\], we propose a \(\delta\)-greedy thresholds to measure the level of greed in orthogonal greedy learning. Our theoretical result shows that orthogonal greedy learning with such a greedy metric yields a learning rate as \(m^{-1/2}(\log m)^2\), which is almost the same as that of the classical SGD-based OGL \[2\]. Thirdly, based on the selected greedy metric, we derive an adaptive terminal rule for the corresponding OGL and thus provide a complete learning system called \(\delta\)-thresholding orthogonal greedy learning (\(\delta\)-TOGL). Lastly, we study the learning performance of \(\delta\)-TOGL in terms of both theoretical analysis and numerical verification. Our study implies that \(\delta\)-TOGL is a competitive learning scheme as the widely used strategies such as the classical orthogonal greedy learning, ridge estimate and lasso estimate. The main results show that when applied to supervised learning problems, \(\delta\)-TOGL outperforms dictionary-based regularization learning schemes such as lasso and ridge regression in the sense that it can produces extremely high sparseness of the final estimator. It also outperforms the classical orthogonal greedy learning in the sense that it provides a more user-friendly parametric selection strategy.

To stimulate more opinions from others on the “greedy-metric” issue of greedy learning, we present the following two remarks.

**Remark 7.1.** In this paper, we give a type of “greedy-metric” for OGL. In greedy approximation, Temlyakov \[32\] has been proposed various greedy-metric such as the super greedy algorithm and weak greedy algorithm. Since greedy learning focus on not only the approximation capability but also the capacity of the space spanned by the selected atoms, we guess that all these metrics can be adopted in greedy learning and may possess similar performances as the classical steepest gradient descent metric. We will also keep working on this issue and report our progress in a future publication.
Remark 7.2. Programmers frequently ask us what is the essential advantage of δ-TOGL. This is a good question and we find a bit headache to answer it. Admittedly, in this paper, we do not provide any essential advantages of δ-TOGL. The purpose of this paper is only to propose the concepts of “greedy metric” and show that we can use the greedy metric to reach the “bias” and “variance” trade-off. However, in our opinion, there are at least two advantages of δ-TOGL. The first one is that, compared with OGL, its generalization capability is not so sensitive to the parameter. This advantage has already been shown in Fig.4 and Fig.5. The second one, δ-TOGL can be viewed as an accelerated version of OGL. As shown in Step 2 in Algorithm 1, we can select the first atom satisfies the greedy metric. Under this circumstance, it need not to compute the $\langle r_{k-1}, g \rangle_m$ for all $g \in D_n$. Once the size of dictionary is large, such an operation can save a large number of computations. As the main purpose of this paper is not to emphasize the computational speed, we do not illustrate this advantage in the present paper. If it is necessary, we will study this advantage within practical applications and report our progress in a future publication.

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