#### Prediction-based Termination Rule for Greedy Learning with Massive Data

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#### Supplementary Material

This supplementary material provides the proofs of Proposition 1 and Theorems 1-2 of the main manuscript. The references cited in this report are listed in the main manuscript.

#### S1 Technical Lemmas

To facilitate our proofs, we first introduce a few technical lemmas. Specifically, let  $\mathcal{G}$  be an arbitrary set of functions (function space). We use  $\mathcal{N}_{\varepsilon}(\mathcal{G}, \nu)$  to denote the covering number of  $\mathcal{G}$  by balls of radius  $\varepsilon$  with respect to a measure  $\nu$ . The lemmas are presented as follows.

**Lemma 1.** Let  $\mathcal{G}$  be a function space defined on a random variable Z. Suppose that, for some constants  $C_1, C_2 \geq 0$ , we have  $|g(Y) - E[g(Y)]| \leq C_1$  and  $E[g(Y)^2] \leq C_2 E[g(Y)]$  for any  $g \in \mathcal{G}$ . Then, for any  $\varepsilon > 0$ ,

$$\mathbf{P}\left\{\sup_{g\in\mathcal{G}}\frac{E[g(Z)] - \frac{1}{n}\sum_{i=1}^{n}g(z_i)}{\sqrt{E[g(Z)] + \varepsilon}} > \sqrt{\varepsilon}\right\} \le \mathcal{N}_{\varepsilon}(\mathcal{G}, \|.\|_{\infty})\exp\left\{-\frac{n\varepsilon}{2C_2 + \frac{2C_1}{3}}\right\},$$

where  $\{z_1, \ldots, z_n\}$  is an i.i.d sample from Z and  $\|.\|_{\infty}$  is the function  $L^{\infty}$  norm.

Lemma 1 is a direct result from Lemma 2 of Zhou and Jetter (2006), which provides a useful probability concentration inequality to bound a function of random variable.

**Lemma 2.** Let  $\mathcal{V}_k$  be a k-dimensional function space defined on  $\mathcal{X}$ . Suppose that there exists a constant T such that  $|v(\boldsymbol{x})| \leq T$  for any  $v \in \mathcal{V}_k$  and  $\boldsymbol{x} \in \mathcal{X}$ . Then

$$\log \mathcal{N}_{\varepsilon}(\mathcal{V}_k, \|.\|_2) \le ck \log \frac{T}{\varepsilon},$$

where c is a positive constant and  $\|.\|_2$  denotes the function  $L^2$  norm.

Lemma 2 is implied by Corollary 2 of Mendelson and Vershinin (2003) together with Property 1 of Maiorov and Ratsaby (1999). It shows that the covering number of a bounded functional space can be also bounded properly.

**Lemma 3.** Let  $\boldsymbol{y} = (y_1, \ldots, y_n)^T$  and  $\hat{f}_k$  be the k-step estimator defined in Algorithm 1. Then, for any  $h \in \text{span}\{D_z^*\}$  and  $k \in \mathbb{N}_n$ ,

$$\|m{y} - \hat{f}_k\|_n^2 \le \|m{y} - h\|_n^2 + rac{4\|h\|_{l_1}^2}{k},$$

where  $||h||_{l_1} = \inf \left\{ \sum_{i=1}^n |\theta_i| : h = \sum_{i=1}^n \theta_i K(\boldsymbol{x}_i, \cdot) / ||K(\boldsymbol{x}_i, \cdot)||_n \right\}.$ 

The proof of Lemma 3 is similar to Theorem 2.3 of Barron et al. (2008). It shows a nice property of the OGA estimator in terms of the empirical approximation error.

## S2 Proof of Proposition 1

Recall that the generalization error of  $\hat{f}_k$  is defined as

$$\mathcal{L}(\hat{f}_k) = \mathcal{E}(\hat{f}_k) - \mathcal{E}(f^*),$$

where  $\mathcal{E}(f) = E(|f(X) - Y|^2)$  for  $f \in \mathcal{F}$ . Let  $\mathcal{E}_n(f) = \|\boldsymbol{y} - f\|_n^2 = \frac{1}{n} \sum_{i=1}^n (y_i - f(\boldsymbol{x}_i))^2$ . Then, for an arbitrary  $h \in \operatorname{span}\{D_z^*\}, \mathcal{L}(\hat{f}_k)$  can be decomposed by

$$\mathcal{L}(\tilde{f}_k) = \mathcal{D} + \mathcal{P} + \mathcal{S},\tag{S2.1}$$

where

$$\mathcal{D} = \mathcal{E}(h) - \mathcal{E}(f^*) = \|h - f^*\|_{\rho_X}^2, \qquad (S2.2)$$
  

$$\mathcal{P} = \mathcal{E}_n(\hat{f}_k) - \mathcal{E}_n(h), \qquad (S2.2)$$
  

$$\mathcal{S} = \mathcal{E}_n(h) - \mathcal{E}(h) + \mathcal{E}(\hat{f}_k) - \mathcal{E}_n(\hat{f}_k).$$

By Lemma 3, we readily have

$$\mathcal{P} \le \frac{4\|h\|_{l_1}^2}{k}.$$
(S2.3)

We proceed to prove the theorem by deriving a probability bound for S. Specifically, we further decompose S by

$$\mathcal{S} = \mathcal{S}_1 + \mathcal{S}_2,\tag{S2.4}$$

where

$$\begin{aligned} \mathcal{S}_1 &= \{\mathcal{E}_n(h) - \mathcal{E}_n(f^*)\} - \{\mathcal{E}(h) - \mathcal{E}(f^*)\}, \\ \mathcal{S}_2 &= \{\mathcal{E}(\hat{f}_k) - \mathcal{E}(f^*)\} - \{\mathcal{E}_n(\hat{f}_k) - \mathcal{E}_n(f^*)\}. \end{aligned}$$

Let us first work on  $S_1$  in (S2.4). Define

$$J(Y,X) = [Y - h(X)]^2 - [Y - f^*(X)]^2$$
  
=  $[f^*(X) - h(X)][2Y - h(X) - f^*(X)].$ 

Clearly, we have

$$\mathcal{S}_1 = \frac{1}{n} \sum_{i=1}^n J(y_i, \boldsymbol{x}_i) - E[J(Y, X)]$$

In our model setup, we assume  $|Y| \leq M$ , which implies that

$$|J| \le (M + ||h||_{\infty})(3M + ||h||_{\infty}) \le (3M + ||h||_{\infty})^{2}.$$

Let  $\xi = (3M + ||h||_{\infty})^2$ . It is then easy to show that

$$|J - E(J)| \le 2\xi \quad \text{and} \quad E(J^2) \le \mathcal{D}\xi \tag{S2.5}$$

with  $\mathcal{D}$  defined in (S2.2). The bounds in (S2.5) together with Bernstein inequality (Shi, Feng, and Zhou (2011)) imply that

$$S_1 \le \frac{4\xi \log \frac{1}{\delta}}{3n} + \sqrt{\frac{2\xi \mathcal{D} \log \frac{1}{\delta}}{n}} \le \frac{7\xi \log \frac{2}{\delta}}{3n} + \frac{\mathcal{D}}{2}$$
(S2.6)

with probability at least  $1 - \delta/2$  for any  $\delta \in (0, 1)$ .

We now turn to bound  $S_2$  in (S2.4). Recall that  $V_k$  in Algorithm 1 is the active set formed by the k basis functions from a k-step OGA procedure. Let  $\mathcal{F}_k = \{T_M[v] : v \in \text{span}\{V_k\}\}$  and g be an arbitrary element from

$$\mathcal{G}_{k} = \left\{ g(X, Y) = \{ f(X) - Y \}^{2} - \{ f^{*}(X) - Y \}^{2}, \ f \in \mathcal{F}_{k} \right\}.$$

Since both |Y| and  $|f^*|$  are bounded by M, it is straightforward to show that  $|g| \leq 8M^2$  and  $|g - E(g)| \leq 16M^2$ . Also, we have

$$E(g^2) = E\left[\{f(X) - f^*(X)\}^2 \{(f(X) - Y) + (f^*(X) - Y)\}^2\right]$$
  
$$\leq 16M^2 E(g).$$

Thus, Lemma 1 becomes applicable to  $\mathcal{G}_k$  with  $C_1 = C_2 = 16M^2$ . Note that

$$E(g) = \mathcal{L}(f) = \mathcal{E}(f) - \mathcal{E}(f^*), \quad \frac{1}{n} \sum_{i=1}^n g(y_i, \boldsymbol{x}_i) = \mathcal{E}_n(f) - \mathcal{E}_n(f^*)$$

for some corresponding  $f \in \mathcal{F}_k$ . This together with Lemma 1 implies that

$$\sup_{f \in \mathcal{F}_k} \left\{ \frac{\mathcal{L}(f) - \{\mathcal{E}_n(f) - \mathcal{E}_n(f^*)\}}{\sqrt{\mathcal{L}(f) + \varepsilon}} \right\} \le \sqrt{\varepsilon}$$
(S2.7)

with probability at least

$$1 - \mathcal{N}_{\varepsilon/4}\left(\mathcal{G}_k, \|.\|_{\infty}\right) \exp\left\{-\frac{3n\varepsilon}{128M^2}\right\}.$$

Note that, for any  $f_1, f_2 \in \mathcal{F}_k$  and the corresponding  $g_1, g_2 \in \mathcal{G}_k$ , we have

$$||g_1 - g_2||_{\infty} = \max_{x,y} |(f_1(x) - y)^2 - (f_2(x) - y)^2|$$
  
$$\leq 4M ||f_1 - f_2||_{\infty},$$

where (x, y) denotes an arbitrary realization from (X, Y). This implies that

$$\mathcal{N}_{\varepsilon/4}\left(\mathcal{G}_{k}, \|.\|_{\infty}\right) \leq \mathcal{N}_{\varepsilon/(16M)}\left(\mathcal{F}_{k}, \|.\|_{\infty}\right)$$
  
$$\leq \mathcal{N}_{\varepsilon/(16M)}\left(\mathcal{F}_{k}, \|.\|_{2}\right)$$
  
$$\leq \exp\left\{ck\log\frac{16M^{2}}{\varepsilon}\right\}, \qquad (S2.8)$$

where the last inequality follows from Lemma 2 with T = M. By (S2.7) and (S2.8), we have

$$P\left\{S_2 \le \frac{1}{2}\mathcal{L}(\hat{f}_k) + \varepsilon\right\} \ge 1 - \exp\left\{ck\log\frac{16M^2}{\varepsilon} - \frac{3n\varepsilon}{128M^2}\right\}.$$
(S2.9)

To further specify (S2.9), let

$$h(\varepsilon) = ck \log \frac{16M^2}{\varepsilon} - \frac{3n\varepsilon}{128M^2}$$

and  $\varepsilon_0$  be the value of  $\varepsilon$  such that  $h(\varepsilon_0) = \log(\delta/2)$  for the same  $\delta$  used in (S2.6). It can be shown that, by choosing

$$\varepsilon_1 = \omega \frac{k \log n + \log \frac{2}{\delta}}{n}$$

with some constant  $\omega > 0$ , we have  $h(\varepsilon_1) \leq h(\varepsilon_0)$ . Since h(.) is a decreasing function, this implies  $\varepsilon_1 \geq \varepsilon_0$ , and therefore

$$P\left\{\mathcal{S}_2 \le \frac{1}{2}\mathcal{L}(\hat{f}_k) + \varepsilon_1\right\} \ge 1 - \delta/2.$$
(S2.10)

Combining the results from (S2.6) and (S2.10), we have

$$P\left\{S \le \frac{\mathcal{D} + \mathcal{L}(\hat{f}_k)}{2} + \frac{7\xi \log \frac{2}{\delta}}{3n} + \varepsilon_1\right\} \ge 1 - \delta.$$
(S2.11)

Inequality (S2.11) together with (S2.2) and (S2.3) further implies that, with probability at least  $1 - \delta$ ,

$$\begin{aligned} \mathcal{L}(\hat{f}_k) &\leq 3\|f^* - h\|_{\rho_X}^2 + \frac{8\|h\|_{l_1}^2}{k} + \frac{14\xi \log \frac{2}{\delta}}{3n} + 2\varepsilon_1 \\ &\leq 3\|f^* - h\|_{\rho_X}^2 + \frac{8\|h\|_{l_1}^2}{k} + \frac{28\log \frac{2}{\delta}\|h\|_{\infty}^2}{3n} + \frac{2\omega k \log n + 6M^2 + \log \frac{2}{\delta}}{n} \end{aligned}$$

Noting  $2\log(2/\delta) > 1$ , we then have, for a sufficiently large n,

$$\begin{aligned} \mathcal{L}(\hat{f}_{k}) &\leq 3\|f^{*} - h\|_{\rho_{X}}^{2} + \frac{16\log\frac{2}{\delta}\|h\|_{l_{1}}^{2}}{k} + \frac{28\log\frac{2}{\delta}\|h\|_{\infty}^{2}}{3n} + \frac{4\omega\log\frac{2}{\delta}k\log n}{n} \\ &\leq C\left[\|f^{*} - h\|_{\rho_{X}}^{2} + \log\frac{2}{\delta}\left(\frac{\|h\|_{l_{1}}^{2}}{k} + \frac{\|h\|_{\infty}^{2}}{n} + \frac{k\log n}{n}\right)\right] \end{aligned}$$

with probability at least  $1-\delta$ , where  $C = \max\{16, 4\omega\}$ . This completes the proof of Proposition 1.

# S3 Proof of Theorem 1

Let  $\mathcal{H}_{\infty} = \lim_{n \to \infty} \operatorname{span}\{D_z^*\}$ . For an arbitrary  $h \in \mathcal{H}_{\infty}$ , we decompose  $\mathcal{L}(\hat{f}_k)$  by

$$\mathcal{L}(\hat{f}_k) = B_1 + B_2 + B_3 + B_4, \tag{S3.1}$$

where

$$B_1 = \|h - \boldsymbol{y}\|_n^2 - \mathcal{E}(h), \quad B_2 = \mathcal{E}(\hat{f}_{k^*}) - \|\hat{f}_k^* - \boldsymbol{y}\|_n^2,$$
  
$$B_3 = \mathcal{E}(h) - \mathcal{E}(f^*), \quad B_4 = \|\hat{f}_k^* - \boldsymbol{y}\|_n^2 - \|h - \boldsymbol{y}\|_n^2.$$

Since  $\mathcal{L}(\hat{f}_k) \geq 0$ , the theorem is proved if

$$P\left\{\lim_{n \to \infty} B_j \le 0\right\} = 1 \tag{S3.2}$$

for j = 1, 2, 3, 4. By the strong law of large numbers, (S3.2) readily holds for  $B_1$ . Thus, it suffices to show (S3.2) for  $B_2$ ,  $B_3$ , and  $B_4$ .

We first show (S3.2) for  $B_2$ . Let

$$\mathcal{G}' = \left\{ g(X, Y) = \left[ f(X) - Y \right]^2 : f \in \mathcal{F}_k \right\}$$

with  $\mathcal{F}_k$  same defined as in the proof of Proposition 1. Since  $|Y| \leq M$ , it is straightforward to show that, for any  $g \in \mathcal{G}'$ ,

$$|g| \le 4M^2$$
,  $|g - E(g)| \le 8M^2$ ,  $E(g^2) \le 4M^2 E(g)$ .

Thus, by applying Lemma 1 to  $\mathcal{G}'$  with  $C_1 = C_2 = 8M^2$  and some arbitrary  $\varepsilon > 0$ , we have

$$\sup_{f \in \mathcal{F}_k} \left\{ \frac{\mathcal{E}(f) - \|f - \boldsymbol{y}\|_n^2}{\sqrt{\mathcal{E}(f) + \varepsilon}} \right\} > \sqrt{\varepsilon}$$
(S3.3)

with probability at most

$$\mathcal{N}_{\varepsilon/4}\left(\mathcal{G}', \|.\|_{\infty}\right) \exp\left\{-\frac{3n\varepsilon}{64M^2}\right\}.$$

Following the same arguments in (S2.8), we have

$$N_{\varepsilon/4}\left(\mathcal{G}', \|.\|_{\infty}\right) \leq \exp\left\{ck\log\frac{16M^2}{\varepsilon}\right\}$$

for some positive constant c. This together with (S3.3) implies that

$$\mathcal{E}(\hat{f}_k) - \|\hat{f}_k - \boldsymbol{y}\|_n^2 > \left[\varepsilon(4M^2 + \varepsilon)\right]^{1/2}$$
(S3.4)

with probability at most

$$P_k = \exp\left\{ck\log\frac{16M^2}{\varepsilon} - \frac{3n\varepsilon}{64M^2}\right\}.$$
(S3.5)

By setting  $k = k^* = T\sqrt{n/\log n}$  with some constant  $T \ge 0$ , we have  $\sum_{n=1}^{\infty} P_{k^*} < \infty$ . Thus, by Borel-Cantelli lemma, (S3.4) and (S3.5) imply that

$$P\left\{\lim_{n \to \infty} B_2 \le \left[\varepsilon(4M^2 + \varepsilon)\right]^{1/2}\right\} = 1.$$
(S3.6)

Since  $\varepsilon$  is arbitrary, (S3.6) further implies that (S3.2) holds for  $B_2$ .

We now proceed to show (S3.2) for  $B_3$  and  $B_4$ . Since  $|f^*(X)| \leq M$ , we have  $||f^*||_{\rho_X} \leq M$ . By Theorem A.1 of Györfy et al. (2002), for any  $\varepsilon' > 0$ , there exists a  $f' \in \mathcal{C}(\mathcal{X})$  such that  $||f' - f^*||_{\rho_X} \leq \varepsilon'$ . Also, Condition C1 implies that  $\mathcal{H}_{\infty}$  is dense in  $\mathcal{H}_K$ . These results together with Condition C2 imply that, for any  $\varepsilon > 0$ , there exists a  $h_{\varepsilon} \in \mathcal{H}_{\infty}$  such that

$$\|h_{\varepsilon} - f^*\|_{\rho_X}^2 \le \varepsilon. \tag{S3.7}$$

By choosing  $h = h_{\varepsilon}$  in (S3.1), we have (S3.2) holds for  $B_3$  due to the arbitrariness of  $\varepsilon$ . Meanwhile, by setting  $k = k^*$ , Lemma 3 implies that

$$B_4 \le \frac{4\|h_{\varepsilon}\|_{l_1}^2}{k^*}.$$
(S3.8)

Since  $D_z^*$  is a normalized dictionary, (S3.7) implies that  $\|h_{\varepsilon}\|_{l_1} < \infty$ . Thus, the right hand side of (S3.8) goes to zero as  $n \to \infty$ , which implies that (S3.2) holds for  $B_4$ . The theorem is therefore proved.

### S4 Proof of Theorem 2

Proposition 1 implies that, for any  $h \in \text{span}\{D_z^*\}$  and n large enough,

$$\mathcal{L}(\hat{f}_k) \le C \left\{ \|f^* - h\|_{\rho_X}^2 + \log \frac{2}{\delta} \left( \frac{\|h\|_{l_1}^2}{k} + \frac{\|h\|_{\infty}^2 + k \log n}{n} \right) \right\}$$

with probability at least  $1 - \delta$  for  $\delta \in (0, 1)$ . When Condition C3 is satisfied with r > 0.5, we have  $\|h'\|_{l_1} \leq B$  and  $\|f^* - h'\|_{\rho_X} \leq \|f^* - h'\|_{\infty} \leq Bn^{-1/2}$  for some  $h' \in \text{span}\{D_z^*\}$ . Since K(.,.) is continues and  $\mathcal{X}$  is compact, Condition C3 also implies that  $\|h'\|_{\infty}^2$  is bounded by some positive constant B'. Based on these results, we have

$$\mathcal{L}(\hat{f}_k) \le C\left\{B^2 n^{-1} + \log\frac{2}{\delta}\left(\frac{B^2}{k} + \frac{B' + k\log n}{n}\right)\right\}$$

with probability at least  $1 - \delta$ . By setting  $k = k^* = T(n/\log n)^{1/2}$ , we have

$$P\left\{\mathcal{L}(\hat{f}_k) > C' \log \frac{2}{\delta} \sqrt{\frac{\log n}{n}}\right\} \le \delta$$

for some generic positive constant C' with a sufficiently large n. Let  $t = C' \log \frac{2}{\delta} (\log n/n)^{1/2}$ , we then have

$$\begin{split} E[\mathcal{L}(\hat{f}_k)] &= \int_0^\infty P\{\mathcal{L}(\hat{f}_k) > t\} dt \\ &\leq \int_0^\infty 2 \exp\left\{-\frac{t}{C'} \sqrt{\frac{n}{\log n}}\right\} dt \\ &\leq 2C' \sqrt{\frac{\log n}{n}}. \end{split}$$

The theorem is therefore proved.