Supplemental Material for Model Free Feature Screening for Ultrahigh-Dimensional Data Conditional on Some Variables

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1 Proof of Step 1

We denote the positive constants c and C as generic constants depending on the context, which can vary from line to line. For simplicity, we write Z(w) with Z for short, where $Z(\cdot)$ is an arbitrary function.

Step 1: For some $0 \le \kappa < 1/2$, we first prove

$$\max_{1 \le j \le p} \sup_{w \in [a,b]} P(|\hat{\rho}^2(X_j, Y|W = w) - \rho^2(X_j, Y|W = w)| \ge cn^{-\kappa}) \le C \exp(-\frac{n^{-\kappa}}{Ch}).$$
(1)

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Define

$$\begin{split} \hat{Z}_{1} &= \frac{1}{n^{2}} \sum_{k,l=1}^{n} K(\frac{W_{k} - w}{h}) K(\frac{W_{l} - w}{h}), \\ \hat{Z}_{2} &= \frac{1}{n^{2}} \sum_{k,l=1}^{n} d_{kl}^{Y} K(\frac{W_{k} - w}{h}) K(\frac{W_{l} - w}{h}), \\ \hat{Z}_{3,j} &= \frac{1}{n^{2}} \sum_{k,l=1}^{n} d_{kl}^{X_{j}} K(\frac{W_{k} - w}{h}) K(\frac{W_{l} - w}{h}), \\ \hat{Z}_{4,j} &= \frac{1}{n^{2}} \sum_{k,l=1}^{n} (d_{kl}^{X_{j}})^{2} K(\frac{W_{k} - w}{h}) K(\frac{W_{l} - w}{h}), \\ \hat{Z}_{5} &= \frac{1}{n^{2}} \sum_{k,l=1}^{n} (d_{kl}^{Y})^{2} K(\frac{W_{k} - w}{h}) K(\frac{W_{l} - w}{h}), \\ \hat{Z}_{6,j} &= \frac{1}{n^{2}} \sum_{k,l=1}^{n} d_{kl}^{X_{j}} d_{kl}^{Y} K(\frac{W_{k} - w}{h}) K(\frac{W_{l} - w}{h}), \\ \hat{Z}_{7} &= \frac{1}{n^{3}} \sum_{k,l=1}^{n} K(\frac{W_{k} - w}{h}) K(\frac{W_{l} - w}{h}), \\ \hat{Z}_{8,j} &= \frac{1}{n^{3}} \sum_{k,l,m=1}^{n} d_{kl}^{X_{j}} d_{km}^{X_{j}} K(\frac{W_{k} - w}{h}) K(\frac{W_{l} - w}{h}), \\ \hat{Z}_{9} &= \frac{1}{n^{3}} \sum_{k,l,m=1}^{n} d_{kl}^{Y} d_{km}^{Y} K(\frac{W_{k} - w}{h}) K(\frac{W_{l} - w}{h}), \\ \hat{Z}_{10,j} &= \frac{1}{n^{3}} \sum_{k,l,m=1}^{n} d_{kl}^{X_{j}} d_{km}^{Y} K(\frac{W_{k} - w}{h}) K(\frac{W_{l} - w}{h}). \end{split}$$

$$\hat{\rho}^{2}(X_{j}, Y|W = w) \text{ can be written as}$$

$$\hat{\rho}^{2}(X_{j}, Y|W = w) = \frac{\hat{Z}_{1}\hat{Z}_{6,j}\hat{Z}_{7}^{2} + \hat{Z}_{2}\hat{Z}_{3,j}\hat{Z}_{7}^{2} - 2\hat{Z}_{1}^{2}\hat{Z}_{7}\hat{Z}_{10,j}}{\sqrt{\hat{Z}_{1}\hat{Z}_{4,j}\hat{Z}_{7}^{2} + \hat{Z}_{3,j}^{2}\hat{Z}_{7}^{2} - 2\hat{Z}_{1}^{2}\hat{Z}_{7}\hat{Z}_{8,j}}\sqrt{\hat{Z}_{1}\hat{Z}_{5}\hat{Z}_{7}^{2} + \hat{Z}_{2}^{2}\hat{Z}_{7}^{2} - 2\hat{Z}_{1}^{2}\hat{Z}_{7}\hat{Z}_{9}}}.$$
(2)

To prove (1), according to Lemma S5 of Liu et al. (2014), we first show

 $\max_{1 \le j \le p} \sup_{w \in [a,b]} P(|\hat{Z}_{6,j} - h^2 f^2(w) E(d_{12}^{X_j} d_{12}^Y | W_1 = w, W_2 = w)| \ge 8cn^{-\kappa}) \le C \exp(-\frac{cn^{-\kappa}}{h}),$

and the other desired inequalities can be obtained analogously.

Define

$$Z_{6,j} = E\hat{Z}_{6,j} = Ed_{kl}^{X_j}d_{kl}^Y K(\frac{W_k - w}{h})K(\frac{W_l - w}{h}),$$

$$\hat{Z}_{6,j}^* = \frac{1}{n(n-1)}\sum_{k\neq l}^n d_{kl}^{X_j}d_{kl}^Y K(\frac{W_k - w}{h})K(\frac{W_l - w}{h}).$$

By condition (C1) and the assumptions in Theorem 1, it can be shown that $\max_{1 \leq j \leq p} \sup_{w \in [a,b]} |Z_{6,j} - h^2 f^2(w) E(d_{12}^{X_j} d_{12}^Y | W_1 = w, W_2 = w)| \leq Ch^3 < 4cn^{-\kappa}$ for large enough *n*. Consequently,

$$\max_{1 \le j \le p} \sup_{w \in [a,b]} P(|\hat{Z}_{6,j} - h^2 f^2(w) E(d_{12}^{X_j} d_{12}^Y | W_1 = w, W_2 = w)| \ge 8cn^{-\kappa})$$

$$\le \max_{1 \le j \le p} \sup_{w \in [a,b]} P(|\hat{Z}_{6,j} - Z_{6,j}| + |Z_{6,j} - h^2 f^2(w) E(d_{12}^{X_j} d_{12}^Y | W_1 = w, W_2 = w)| \ge 8cn^{-\kappa})$$

$$\le \max_{1 \le j \le p} \sup_{w \in [a,b]} P(|\hat{Z}_{6,j} - Z_{6,j}| \ge 4cn^{-\kappa}). \tag{3}$$

By using the Cauchy-Schwartz inequality and condition (C2), it follows

$$Z_{6,j} \le M_0^2 E |d_{kl}^{X_j} d_{kl}^Y| \le M_0^2 (E(d_{kl}^{X_j})^2 E(d_{kl}^Y)^2)^{1/2},$$

where $|K(t)| \leq M_0 < \infty$ hold uniformly over the support of $K(\cdot)$. This, together with condition (C3), implies that $Z_{6,j}$ is uniformly bounded in p. That is, $\max_{1 \leq j \leq p} Z_{6,j} < \infty$. Take n large enough such that $Z_{6,j}/n < 2cn^{-\kappa}$. Then, it can be easily shown that

$$\max_{1 \le j \le p} \sup_{w \in [a,b]} P(|\hat{Z}_{6,j} - Z_{6,j}| \ge 4cn^{-\kappa}) \\
= \max_{1 \le j \le p} \sup_{w \in [a,b]} P(|\hat{Z}_{6,j}^* \frac{n-1}{n} - Z_{6,j} \frac{n-1}{n} - Z_{6,j} \frac{1}{n}| \ge 4cn^{-\kappa}) \\
\le \max_{1 \le j \le p} \sup_{w \in [a,b]} P(|\hat{Z}_{6,j}^* - Z_{6,j}| \frac{n-1}{n} \ge 4cn^{-\kappa} - Z_{6,j} \frac{1}{n}) \\
\le \max_{1 \le j \le p} \sup_{w \in [a,b]} P(|\hat{Z}_{6,j}^* - Z_{6,j}| \ge 2cn^{-\kappa}).$$
(4)

To establish the uniform consistency of $\hat{Z}_{6,j}$ in j, it suffices to show the uniform consistency of $\hat{Z}_{6,j}^*$ in j. Let $h(X_{jk}, Y_k, W_k; X_{jl}, Y_l, W_l; w) = d_{kl}^{X_j} d_{kl}^Y K(\frac{W_k - w}{h}) K(\frac{W_l - w}{h}) := hI(h > M) + hI(h \le M)$ be the kernel of the U statistics $\hat{Z}_{6,j}^*$, where M will be specified later. Then

$$\begin{split} \hat{Z}^*_{6,j} &= \quad \frac{1}{n(n-1)} \sum_{k \neq l}^n hI(h \le M) + \frac{1}{n(n-1)} \sum_{k \neq l}^n hI(h > M) \\ &:= \quad \hat{Z}^*_{61,j} + \hat{Z}^*_{62,j}. \end{split}$$

Accordingly, we decompose the $Z_{6,j}$ into

$$Z_{6,j} = EhI(h \le M) + EhI(h > M) := Z_{61,j} + Z_{62,j}.$$

We prove the uniform consistency of $\hat{Z}_{61,j}^*$ in j, first, with the Markov's inequality, for any t > 0, we have

$$P(\hat{Z}_{61,j}^* - Z_{61,j} \ge cn^{-\kappa}) \le \exp(-tcn^{-\kappa})\exp(-tZ_{61,j})E\exp(t\hat{Z}_{61,j}^*).$$
(5)

With a similar discussion about U statistics in Zhu et al. (2011), the U statistics $\hat{Z}_{61,j}^*$ can be represented as an average of iid random variables. That is,

$$\hat{Z}_{61,j}^* = (n!)^{-1} \sum_{n!} \Omega(X_{j1}, Y_1, W_1; \cdots; X_{jn}, Y_n, W_n, w),$$

where $\sum_{n!}$ denotes the summation over all possible permutations of $(1, 2, \dots, n)$, and each $\Omega(X_{j1}, Y_1; \dots; X_{jn}, Y_n)$ is an average of $m = \lfloor n/2 \rfloor$ iid random variables. Thus, it follows from the Jensen's inequality that, for $j = 1, 2, \dots, p$,

$$E \exp(t\hat{Z}_{61,j}^{*}) = E \exp(t(n!)^{-1} \sum_{n!} \Omega(X_{j1}, Y_1, W_1; \cdots; X_{jn}, Y_n, W_n, w))$$

$$\leq (n!)^{-1} \sum_{n!} E \exp(t\Omega(X_{j1}, Y_1, W_1; \cdots; X_{jn}, Y_n, W_n, w))$$

$$= E^m \exp(tm^{-1}hI(h \le M)).$$
(6)

According to Lemma 1 in Li et al. (2012), for $j = 1, 2, \dots, p$, by (5), (6), we have

$$P(\hat{Z}_{61,j}^* - Z_{61,j} \ge cn^{-\kappa}) \le \exp(-tcn^{-\kappa})E^m \exp(m^{-1}t[hI(h \le M) - Z_{61,j}])$$
$$\le \exp(-tcn^{-\kappa} + M^2t^2/8m).$$

By choosing $t = 4cn^{-\kappa}m/M^2$ such that $P(\hat{Z}_{61,j}^* - Z_{61,j} \ge cn^{-\kappa}) \le \exp(-2c^2n^{-2\kappa}m/M^2)$. Similarly, we can prove that $P(\hat{Z}_{61,j}^* - Z_{61,j} \le -cn^{-\kappa}) \le \exp(-2c^2n^{-2\kappa}m/M^2)$. Therefore, for $j = 1, 2, \cdots, p$, we have

$$P(|\hat{Z}_{61,j}^* - Z_{61,j}| \ge cn^{-\kappa}) \le 2\exp(-2c^2n^{-2\kappa}m/M^2) = 2\exp(-\frac{cn^{-\kappa}}{h}\frac{2cn^{-\kappa}mh}{M^2}).$$
 (7)

Since $h = O(n^{-\gamma})$, we take $M = O(n^{\tau})$, where $\gamma - \kappa < \tau < (1 - \gamma - \kappa)/2$, such that

$$\frac{2cn^{-\kappa}mh}{M^2} = Cn^{1-\gamma-\kappa-2\tau} > 1,$$

for sufficiently large n. (7) is then simplified as

$$P(|\hat{Z}_{61,j}^* - Z_{61,j}| \ge cn^{-\kappa}) \le C \exp(-\frac{cn^{-\kappa}}{h}).$$
(8)

Next, we consider the uniform consistency of $\hat{Z}^*_{62,j}$ in j, with Cauchy-Schwartz inequality and Markov's inequality, we have

$$Z_{62,j}^2 \leq E(h^2)P(h > M) \leq E(h^2)\exp(-s'M)E(\exp(s'h))$$
 for $0 < s' < s_0$.

By some simple inequalities, we have

$$h = \{ (X_{jk} - X_{jl})^2 (Y_k - Y_l)^\top (Y_k - Y_l) K^2 (\frac{w_k - w}{h}) K^2 (\frac{w_l - w}{h}) \}^{1/2}$$

$$\leq 2M_0^2 \{ (X_{jk}^2 + X_{jl}^2) (Y_k^2 + Y_l^2) \}^{1/2}$$

$$\leq M_0^2 \{ (X_{jk}^2 + X_{jl}^2 + Y_k^2 + Y_l^2)^2 \}^{1/2}$$

$$\leq M_0^2 (X_{jk}^2 + X_{jl}^2 + Y_k^2 + Y_l^2),$$

which yields that

$$E(\exp(s'h)) \le E(\exp(s'M_0^2(X_{jk}^2 + X_{jl}^2 + Y_k^2 + Y_l^2))).$$

By condition (C3), and notice that $M = O(n^{\tau})$, then $\max_{1 \le j \le p} Z_{62,j} < cn^{-\kappa}/2$ when n is sufficiently large. Thus, for $j = 1, 2, \cdots, p$, we get

$$\begin{split} P(|\hat{Z}_{62,j}^* - Z_{62,j}| > cn^{-\kappa}) &\leq P(|\hat{Z}_{62,j}^*| > cn^{-\kappa}/2) \\ &\leq P(X_{ji}^2 + Y_i^2 > M/(2M_0^2), \text{ for some } 1 \leq i \leq n) \\ &\leq nP(X_{ji}^2 > M/(4M_0^2)) + nP(Y_i^2 > M/(4M_0^2)) \\ &\leq 2nC \exp(-sM/(4M_0^2)) \\ &= 2C \exp(-\frac{cn^{-\kappa}}{h}\frac{h(sM/(4M_0^2) - \log n)}{cn^{-\kappa}}). \end{split}$$

The second line is because that if $X_{ji}^2 + Y_i^2 \leq M/(2M_0^2)$ for all $1 \leq i \leq n$, we then have $h \leq M_0^2(X_{jk}^2 + X_{jl}^2 + Y_k^2 + Y_l^2) \leq M$. This leads to $|\hat{Z}_{62,j}^*| = 0$, which contradict with $|\hat{Z}_{62,j}^*| > cn^{-\kappa}/2$. The fourth line is due to Markov's inequality and condition (C3). Since $\frac{h(sM/(4M_0^2) - \log n)}{cn^{-\kappa}} = C(n^{\kappa+\tau-\gamma} - n^{\kappa-\gamma}\log n) > 1$, then, for $j = 1, 2, \cdots, p$, we have

$$P(|\hat{Z}_{62,j}^* - Z_{62,j}| > cn^{-\kappa}) \le C \exp(-\frac{cn^{-\kappa}}{h}).$$
(9)

Summarizing equations (3), (4), (8), (9), we obtain

 $\max_{1 \le j \le p} \sup_{w \in [a,b]} P(|\hat{Z}_{6,j} - h^2 f^2(w) E(d_{12}^{X_j} d_{12}^Y | W_1 = w, W_2 = w)| \ge 8cn^{-\kappa}) \le C \exp(-\frac{cn^{-\kappa}}{h}).$

2 Additional simulation

Following Example 3 in Fan et al. (2014), we further consider a linear varying coefficient model setup. Let $\{Z_1, \dots, Z_p\}$ be iid standard normal, $\{U_1, U_2\}$ be iid standard uniformly distributed random variables, and the noise ϵ follows the standard normal distribution. The model is specified as:

$$Y = 2X_1 + 3WX_2 + (W+1)^2 X_3 + \frac{4\sin(2\pi W)}{2 - \sin 2\pi W} X_4 + \epsilon,$$

where $X_j = (Z_j + t_1U_1)/(1 + t_1)$, $j = 1, \dots, p$ and $W = (U_2 + t_2U_1)/(1 + t_2)$. t_1, t_2 controls the correlation among the predictors **X** and the correlation between **X** and *W* respectively. We study one setting: $t_1 = t_2 = 0$, which results in uncorrelated case.

We take p to be 1000, and the sample size n is 200, the model size d is chosen to be $d_i = i[n^{4/5}/log(n^{4/5})]$, i = 1, 2, 3, where [a] denotes the integer part of a. Let $0 = s_0 < s_1 < \cdots < s_{10} < s_{11} = 1$ be a partition of the interval. Using the s_i as knots, we construct 7 normalized cubic (order is 3) B-spline basis functions for NIS method. All the simulations are based on 500 replications. Similarly, we report the S, P_j and P_{All} in Table 1-2. We further present the boxplot of S in Figure 1.

Insert Table 1-2, Figure 1 here

Based on the results in Table 1-2 and Figure 1, we can see that in this uncorrelated case, CDC-SIS, CC-SIS, NIS perform well and behave better than the unconditional screening methods SIS, DC-SIS and DC-RoSIS. NIS behave comparable to the CDC-SIS and CC-SIS according to the top fifty percent quantiles of S. However, in terms of the 75% and 95% quantiles of S, NIS method need a larger model size to include all active predictors than the CDC-SIS and CC-SIS methods. Moreover, P_{All} of NIS is a little lower than those of CDC-SIS and CC-SIS, but all these three methods outperform the unconditional screening methods significantly.

References

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Table 1: The quantile of S

t_1, t_2	method	5%	25%	50%	75%	95%
$t_1 = t_2 = 0$	CDC-SIS	4.0000	4.0000	4.0000	4.0000	5.0000
	CC-SIS	4.0000	4.0000	4.0000	4.0000	5.0000
	NIS	4.0000	4.0000	5.0000	13.0000	74.0000
	SIS	4.0000	6.0000	25.5000	102.0000	410.5000
	DC-SIS	4.0000	7.0000	28.0000	114.0000	427.5000
	DC-RoSIS	4.0000	7.0000	31.0000	138.0000	472.5000

Table 2: The proportion of P_j and P_{All}

				P_{All}			
t_{1}, t_{2}	method	size	X_1	X_2	X_3	X_4	All
$t_1 = t_2 = 0$	CDC-SIS	d_1	1.0000	0.9880	1.0000	1.0000	0.9880
		d_2	1.0000	0.9960	1.0000	1.0000	0.9960
		d_3	1.0000	0.9960	1.0000	1.0000	0.9960
	CC-SIS	d_1	1.0000	0.9980	1.0000	1.0000	0.9980
		d_2	1.0000	0.9980	1.0000	1.0000	0.9980
		d_3	1.0000	0.9980	1.0000	1.0000	0.9980
	NIS	d_1	0.9860	0.8120	1.0000	0.9920	0.7940
		d_2	0.9980	0.8860	1.0000	0.9980	0.8840
		d_3	1.0000	0.9260	1.0000	1.0000	0.9260
	SIS	d_1	1.0000	0.9980	1.0000	0.4160	0.4140
		d_2	1.0000	1.0000	1.0000	0.5340	0.5340
		d_3	1.0000	1.0000	1.0000	0.6180	0.6180
	DC-SIS	d_1	1.0000	0.9900	1.0000	0.4100	0.4060
		d_2	1.0000	0.9960	1.0000	0.5260	0.5240
		d_3	1.0000	0.9980	1.0000	0.5980	0.5960
	DC-RoSIS	d_1	1.0000	0.9800	1.0000	0.3840	0.3780
		d_2	1.0000	0.9920	1.0000	0.5080	0.5060
		d_3	1.0000	0.9940	1.0000	0.5760	0.5740

Figure 1: Boxplot of minimum model size



(a) $t_1 = t_2 = 0$