Statistical Inference after Kernel Ridge Regression Imputation under item nonresponse

Hengfang Wang         Jae Kwang Kim

Abstract

Imputation is a popular technique for handling missing data. We consider a nonparametric approach to imputation using the kernel ridge regression technique and propose consistent variance estimation. The proposed variance estimator is based on a linearization approach which employs the entropy method to estimate the density ratio. The $\sqrt{n}$-consistency of the imputation estimator is established when a Sobolev space is utilized in the kernel ridge regression imputation, which enables us to develop the proposed variance estimator. Synthetic data experiments are presented to confirm our theory.

Key words: Reproducing kernel Hilbert space; Missing data; Nonparametric method
1 Introduction

Missing data is a universal problem in statistics. Ignoring the cases with missing values can lead to misleading results ([Kim and Shao 2013; Little and Rubin 2019]). To avoid the potential problem with missing data, imputation is commonly used. After imputation, the imputed dataset can serve as a complete dataset that has no missing values, which in turn makes results from different analysis methods consistent. However, treating imputed data as if observed and applying the standard estimation procedure may result in misleading inference, leading to underestimation of the variance of imputed point estimators. As a result, how to make statistical inferences with imputed point estimators is an important statistical problem. An overview of imputation method can be found in [Haziza 2009].

Multiple imputation, proposed by [Rubin 2004], addresses the uncertainty associated with imputation. However, variance estimation using Rubin’s formula requires certain conditions ([Wang and Robins 1998; Kim et al. 2006; Yang and Kim 2016]), which do not necessarily hold in practice. An alternative method is fractional imputation, originally proposed by [Kalton and Kish 1984]. The main idea of fractional imputation is to generate multiple imputed values and the corresponding fractional weights. In particular, [Kim 2011] and [Kim and Yang 2014] employ fully parametric approach to handling nonresponse items with fractional imputation. However, such parametric fractional imputation relies heavily on the parametric model assumptions. To mitigate the effects of parametric model assumption, empirical likelihood ([Owen 2001; Qin and Lawless 1994]) as a semi-parametric approach was considered. In particular, [Wang and Chen 2009] employed the kernel smoothing approach to do empirical likelihood inference with missing values. [Cheng 1994] utilized the kernel-based nonparametric regression
approach to do the imputation and established the $\sqrt{n}$-consistency of the imputed estimator.

Kernel ridge regression (Friedman et al., 2001; Shawe-Taylor et al., 2004) is a popular data-driven approach which can alleviate the effect of model assumption. By using a regularized $M$-estimator in reproducing kernel Hilbert space (RKHS), kernel ridge regression can capture the model with complex reproducing kernel Hilbert space while a regularized term makes the original infinite dimensional estimation problem viable (Wahba, 1990; van de Geer, 2000; Mendelson, 2002; Zhang, 2005; Koltchinskii et al., 2006; Steinwart et al., 2009) studied the error bounds for the estimates of kernel ridge regression method.

In this paper, we apply kernel ridge regression as a nonparametric imputation method and propose a consistent variance estimator for the corresponding imputation estimator under missing at random framework. Because the kernel ridge regression is a general tool for nonparametric regression with flexible assumptions, the proposed imputation method is practically useful. Variance estimation after the kernel ridge regression imputation is a challenging but important problem. To the best of our knowledge, this is the first paper which considers kernel ridge regression technique and discusses its variance estimation in the imputation framework. Specifically, we first prove $\sqrt{n}$-consistency of the kernel ridge regression imputation estimator and obtain influence function for linearization. After that, we employ the maximum entropy method (Nguyen et al., 2010) for density ratio estimation to get a valid estimate of the inverse of the propensity scores. The consistency of our variance estimator can then be established.

The paper is organized as follows. In Section 2, the basic setup and the proposed method are introduced. In Section 3, main theory is established. We also in-
introduce a novel nonparametric estimator of the propensity score function. Results from two limited simulation studies are presented in Section 4. An illustration of the proposed method to a real data example is presented in Section 5. Some concluding remarks are made in Section 6.

2 Proposed Method

Consider the problem of estimating $\theta = \mathbb{E}(Y)$ from an independent and identically distributed (IID) sample $\{(x_i, y_i), i = 1, \ldots, n\}$ of random vector $(X, Y)$. Instead of always observing $y_i$, suppose that we observe $y_i$ only if $\delta_i = 1$, where $\delta_i$ is the response indicator function of unit $i$ taking values on $\{0, 1\}$. The auxiliary variable $x_i$ are always observed. We assume that the response mechanism is missing at random (MAR) in the sense of Rubin (1976).

Under MAR, we can develop a nonparametric estimator $\hat{m}(x)$ of $m(x) = \mathbb{E}(Y \mid x)$ and construct the following imputation estimator:

$$\hat{\theta}_I = \frac{1}{n} \sum_{i=1}^{n} \left\{ \delta_i y_i + (1 - \delta_i) \hat{m}(x_i) \right\}.$$  \hspace{1cm} (1)

If $\hat{m}(x)$ is constructed by the kernel-based nonparametric regression method, we can express

$$\hat{m}(x) = \frac{\sum_{i=1}^{n} \delta_i K_h(x_i, x) y_i}{\sum_{i=1}^{n} \delta_i K_h(x_i, x)} \hspace{1cm} (2)$$

where $K_h(\cdot)$ is the kernel function with bandwidth $h$. Under some suitable choice of the bandwidth $h$, Cheng (1994) first established the $\sqrt{n}$-consistency of the imputation estimator (1) with nonparametric function in (2). However, the kernel-based regression imputation in (2) is applicable only when the dimension of $x$ is small.
In this paper, we extend the work of Cheng (1994) by considering a more general type of the nonparametric imputation, called kernel ridge regression (KRR) imputation. The KKR technique can be understood using the reproducing kernel Hilbert space (RKHS) theory (Aronszajn, 1950) and can be described as

$$\hat{m} = \arg \min_{m \in \mathcal{H}} \left[ \sum_{i=1}^{n} \delta_i \{ y_i - m(x_i) \}^2 + \lambda \| m \|_{\mathcal{H}}^2 \right], \quad (3)$$

where $\| m \|_{\mathcal{H}}^2$ is the norm of $m$ in the Hilbert space $\mathcal{H}$. Here, the inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ is induced by such a kernel function, i.e.,

$$\langle f, K(\cdot, x) \rangle_{\mathcal{H}} = f(x), \quad \forall x \in \mathcal{X}, \; f \in \mathcal{H}, \quad (4)$$

namely, the reproducing property of $\mathcal{H}$. Naturally, this reproducing property implies the $\mathcal{H}$ norm of $f$: $\| f \|_{\mathcal{H}} = \langle f, f \rangle_{\mathcal{H}}^{1/2}$.

One canonical example of such a space is the Sobolev space. Specifically, assuming that the domain of such functional space is $[0, 1]$, the Sobolev space of order $l$ can be denoted as

$$\mathcal{W}^l_2 = \left\{ f : [0, 1] \rightarrow \mathbb{R} | f, f^{(1)}, \ldots, f^{(l-1)} \text{ are absolute continuous and } f^{(l)} \in L^2[0, 1] \right\}.$$ 

One possible norm for this space can be

$$\| f \|_{\mathcal{W}^l_2}^2 = \sum_{q=0}^{l-1} \left\{ \int_0^1 f^{(q)}(t) dt \right\}^2 + \int_0^1 \left\{ f^{(l)}(t) \right\}^2 dt.$$

In this section, we employ the Sobolev space of second order as the approximation space. For Sobolev space of order $\ell$, we have the kernel function

$$K(x, y) = \sum_{q=0}^{\ell-1} k_q(x)k_q(y) + k_\ell(x)k_\ell(y) + (-1)^\ell k_{2\ell}(|x - y|),$$

One possible norm for this space can be

$$\| f \|_{\mathcal{W}^\ell_2}^2 = \sum_{q=0}^{\ell-1} \left\{ \int_0^1 f^{(q)}(t) dt \right\}^2 + \int_0^1 \left\{ f^{(\ell)}(t) \right\}^2 dt.$$
where \( k_q(x) = (q!)^{-1} B_q(x) \) and \( B_q(\cdot) \) is the Bernoulli polynomial of order \( q \).

By the representer theorem for RKHS (Wahba, 1990), the estimate in (3) lies in the linear span of \( \{K(\cdot, x_i), i = 1, \ldots, n\} \). Specifically, we have

\[
\hat{m}(\cdot) = \sum_{i=1}^{n} \hat{\alpha}_{i,\lambda} K(\cdot, x_i),
\]

where

\[
\hat{\alpha}_{\lambda} = (\Delta_n K + \lambda I_n)^{-1} \Delta_n y,
\]

\( \Delta_n = \text{diag}(\delta_1, \ldots, \delta_n) \), \( K = (K(x_i, x_j))_{ij} \), \( y = (y_1, \ldots, y_n)^T \) and \( I_n \) is the \( n \times n \) identity matrix.

The tuning parameter \( \lambda \) is selected via generalized cross-validation (GCV) in KRR, where the GCV criterion for \( \lambda \) is

\[
\text{GCV}(\lambda) = \frac{n^{-1} \| \{\Delta_n - A(\lambda)\} y \|^2}{n^{-1} \text{Trace}(\Delta_n - A(\lambda))},
\]

(6)

and \( A(\lambda) = \Delta_n K(\Delta_n K + \lambda I_n)^{-1} \Delta_n \). The value of \( \lambda \) minimizing the GCV is used for the selected tuning parameter.

Using the KRR imputation in (3), we aim to establish the following two goals:

1. Find the sufficient conditions for the \( \sqrt{n} \)-consistency of the imputation estimator \( \hat{\theta}_I \) using (5) and give a formal proof.

2. Find a linearization variance formula for the imputation estimator \( \hat{\theta}_I \) using the KRR imputation.

The first part is formally presented in Theorem 1 in Section 3. For the second part, we employ the density ratio estimation method of Nguyen et al. (2010) to get a consistent estimator of \( \omega(x) = \{\pi(x)\}^{-1} \) in the linearized version of \( \hat{\theta}_I \).
3 Main Theory

Before we develop our main theory, we first introduce Mercer’s theorem.

**Lemma 1** (Mercer’s theorem). *Given a continuous, symmetric, positive definite kernel function* $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$. *For* $x, z \in \mathcal{X}$, *under some regularity conditions, Mercer’s theorem characterizes* $K$ *by the following expansion*

$$K(x, z) = \sum_{j=1}^{\infty} \lambda_j \phi_j(x) \phi_j(z),$$

*where* $\lambda_1 \geq \lambda_2 \geq \ldots \geq 0$ *are a non-negative sequence of eigenvalues and* $\{\phi_j\}_{j=1}^{\infty}$ *is an orthonormal basis for* $L^2(\mathbb{P})$.

To develop our theory, we make the following assumptions.

[A1] For some $k \geq 2$, there is a constant $\rho < \infty$ such that $E[\phi_j(x)^{2k}] \leq \rho^{2k}$ for all $j \in \mathbb{N}$, where $\{\phi_j\}_{j=1}^{\infty}$ are orthonormal basis by expansion from Mercer’s theorem.

[A2] The function $m \in \mathcal{H}$, and for $x \in \mathcal{X}$, we have $E[\{Y - m(x)\}^2] \leq \sigma^2$, for some $\sigma^2 < \infty$.

[A3] The propensity score $\pi(\cdot)$ is uniformly bounded away from zero. In particular, there exists a positive constant $c > 0$ such that $\pi(x_i) \geq c$, for $i = 1, \ldots, n$.

[A4] The ratio $d/\ell < 2$ for $d$-dimensional Sobolev space of order $\ell$, where $d$ is the dimension of covariate $x$.

The first assumption is a technical assumption which controls the tail behavior of $\{\phi_j\}_{j=1}^{\infty}$. Assumption 2 indicates that the noises have bounded variance.
Assumption 1 and Assumption 2 together aim to control the error bound of the kernel ridge regression estimate \( \hat{m} \). Furthermore, Assumption 3 means that the support for the respondents should be the same as the original sample support. Assumption 3 is a standard assumption for missing data analysis. Assumption 4 is a technical assumption for entropy analysis. Intuitively, when the dimension is large, the Sobolev space should be large enough to capture the true model.

**Theorem 1.** Suppose Assumption 1 \( \sim 4 \) hold for a Sobolev kernel of order \( \ell \), \( \lambda = n^{1-\ell} \), we have

\[
\sqrt{n}(\hat{\theta}_I - \bar{\theta}_I) = o_p(1),
\]

where

\[
\bar{\theta}_I = \frac{1}{n} \sum_{i=1}^{n} \left[ m(x_i) + \delta_i \frac{1}{\pi(x_i)} \{ y_i - m(x_i) \} \right]
\]

and

\[
\sqrt{n} \left( \bar{\theta}_I - \theta \right) \overset{\mathcal{L}}{\longrightarrow} N(0, \sigma^2),
\]

with

\[
\sigma^2 = V\{E(Y \mid x)\} + E\{V(Y \mid x)/\pi(x)\}.
\]

Theorem [1] guarantees the asymptotic equivalence of \( \hat{\theta}_I \) and \( \bar{\theta}_I \) in (8). Specifically, the reference distribution is a combination of an outcome model and a propensity score model for sampling mechanism. The variance of \( \bar{\theta}_I \) achieves the semiparametric lower bound of [Robins et al., 1994]. The proof of Theorem [1] is presented in the Appendix.

The linearization formula in (8) can be used for variance estimation. The idea is to estimate the influence function \( \eta_i = m(x_i) + \delta_i (\pi(x_i))^{-1} \{ y_i - m(x_i) \} \)
and apply the standard variance estimator using \( \hat{\eta}_i \). To estimate \( \eta_i \), we need an estimator of \( \pi(x) \). We propose a version of KRR method to estimate \( \omega(x) = \{\pi(x)\}^{-1} \) directly. In order to estimate \( \omega(x) = \{\pi(x)\}^{-1} \), we wish to develop a KRR version of estimating \( \omega(x) \). To do this, first define

\[
g(x) = \frac{f(x \mid \delta = 0)}{f(x \mid \delta = 1)},
\]

and, by Bayes theorem, we have

\[
\omega(x) = \frac{1}{\pi(x)} = 1 + \frac{n_0}{n_1} g(x).
\]

Thus, to estimate \( \omega(x) \), we have only to estimate the density ration function \( g(x) \) in (9). Now, to estimate \( g(x) \) nonparametrically, we use the idea of Nguyen et al. (2010) for the KRR approach to density ratio estimation.

To explain the KRR estimation of \( g(x) \), note that \( g(x) \) can be understood as the maximizer of

\[
Q(g) = \int \log(g) f(x \mid \delta = 0) d\mu(x) - \int g(x) f(x \mid \delta = 1) d\mu(x)
\]

with constraint

\[
\int g(x) f(x \mid \delta = 1) d\mu(x) = 1.
\]

The sample version objective function is

\[
\hat{Q}(g) = \frac{1}{n_0} \sum_{i=1}^{n} \mathbb{I}(\delta_i = 0) \log\{g(x_i)\} - \frac{1}{n_1} \sum_{i=1}^{n} \mathbb{I}(\delta_i = 1) g(x_i)
\]

where \( n_k = \sum_{i=1}^{n} \mathbb{I}(\delta_i = k) \). The maximizer of \( \hat{Q}(g) \) is an M-estimator of the density ratio function \( g \).

Further, define \( h(x) = \log\{g(x)\} \). The loss function \( L(\cdot) \) derived from the optimization problem in (11) can be written as

\[
L(\delta, h(x)) = \frac{1}{n_1} \mathbb{I}(\delta = 1) \exp\{h(x)\} - \frac{1}{n_0} \mathbb{I}(\delta = 0) h(x).
\]
In our problem, we wish to find $h$ that minimizes
\[
\sum_{i=1}^{n} L(\delta_i, \alpha_0 + h(x_i)) + \tau \|h\|_H^2
\] (12)
over $\alpha_0 \in \mathbb{R}$ and $h \in \mathcal{H}$, where $L(\cdot)$ is the loss function derived from the optimization problem in (10) using maximum entropy.

Hence, using the representer theorem again, the solution to (12) can be obtained as
\[
\min_{\alpha \in \mathbb{R}^n} \left\{ \sum_{i=1}^{n} L(\delta_i, \alpha_0 + \sum_{j=1}^{n} \alpha_j K(x_i, x_j)) + \tau \alpha'K\alpha \right\}
\] (13)
and $\alpha_0$ is a normalizing constant satisfying
\[
n_1 = \sum_{i=1}^{n} \mathbb{I}(\delta_i = 1) \exp\{\alpha_0 + \sum_{j=1}^{n} \hat{\alpha}_j K(x_i, x_j)\}.
\]
Thus, we use
\[
\hat{g}(x) = \exp\{\hat{\alpha}_0 + \sum_{j=1}^{n} \hat{\alpha}_j K(x, x_j)\}
\] (14)
as a nonparametric approximation of the density ratio function $g(x)$. Also,
\[
\hat{\omega}(x) = 1 + \frac{n_0}{n_1} \hat{g}(x)
\] (15)
is the nonparametric approximation of $\omega(x) = \{\pi(x)\}^{-1}$. Note that $\tau$ is the tuning parameter that determines the model complexity of $g(x)$. The tuning parameter selection is discussed in Appendix B.

Therefore, we can use
\[
\hat{V} = \frac{1}{n^2} \frac{1}{n-1} \sum_{i=1}^{n} (\hat{\eta}_i - \bar{\eta}_n)^2
\] (16)
as a variance estimator of $\hat{\theta}$, where
\[
\hat{\eta}_i = \hat{m}(x_i) + \delta_i \hat{\omega}_i(x_i) \{y_i - \hat{m}(x_i)\}
\] (17)
and $\bar{\eta}_n = n^{-1} \sum_{i=1}^{n} \hat{\eta}_i$. 

10
4 Simulation Study

4.1 Simulation study one

To evaluate the performance of the proposed imputation method and its variance estimator, we conduct two simulation studies. In the first simulation study, a continuous study variable is considered with three different data generating models. In the three models, we keep the response rate around 70% and $\text{Var}(Y) \approx 10$. Also, $\mathbf{x}_i = (x_{i1}, x_{i2}, x_{i3}, x_{i4})^T$ are generated independently element-wise from the uniform distribution on the support $(1, 3)$. In the first model (Model A), we use a linear regression model

$$y_i = 3 + 2.5x_{i1} + 2.75x_{i2} + 2.5x_{i3} + 2.25x_{i4} + \sigma \epsilon_i,$$

to obtain $y_i$, where $\{\epsilon_i\}_{i=1}^n$ are generated from standard normal distribution and $\sigma = \sqrt{3}$. In the second model (Model B), we use

$$y_i = 3 + (1/35)x_{i1}^2x_{i2}^3x_{i3} + 0.1x_{i4} + \epsilon_i$$

to generate data with a nonlinear structure. The third model (Model C) for generating the study variable is

$$y_i = 3 + (1/180)x_{i1}^2x_{i2}^3x_{i3}^2x_{i4}^2 + \epsilon_i.$$

In addition to $\{(x_i^T, y_i)^T, i = 1, \ldots, n\}$, the response indicator variable $\delta$’s are independently generated from the Bernoulli distribution with probability $\text{logit}(x_i'\beta + 2.5)$, where $\beta = (-1, 0.5, -0.25, -0.1)^T$ and $\text{logit}(p) = \log\{p/(1-p)\}$. We considered three sample sizes $n = 200, n = 500$ and $n = 1,000$ with 1,000 Monte Carlo replications. The reproducing kernel Hilbert space we employed is the second-order Sobolev space.
We also compare three imputation methods: kernel ridge regression (KRR), B-spline, linear regression (Linear). We compute the Monte Carlo biases, variance, and the mean squared errors of the imputation estimators for each case. The corresponding results are presented in Table 1.

Table 1: Biases, Variances and Mean Squared Errors (MSEs) of three imputation estimators for continuous responses

| Model | Sample Size | Criteria | KRR     | B-spline | Linear |
|-------|-------------|----------|---------|----------|--------|
|       |             | Bias     | -0.0577 | 0.0027   | 0.0023 |
|       |             | Var      | 0.0724  | 0.0679   | 0.0682 |
|       |             | MSE      | 0.0757  | 0.0679   | 0.0682 |
| A     | 200         | Bias     | -0.0358 | 0.0038   | 0.0038 |
|       |             | Var      | 0.0275  | 0.0263   | 0.0263 |
|       |             | MSE      | 0.0288  | 0.0263   | 0.0263 |
|       | 500         | Bias     | -0.0292 | 0.0002   | 0.0002 |
|       |             | Var      | 0.0132  | 0.0128   | 0.0129 |
|       |             | MSE      | 0.0141  | 0.0128   | 0.0129 |
|       | 1000        | Bias     | -0.0188 | 0.0493   | 0.0372 |
|       |             | Var      | 0.0644  | 0.0674   | 0.0666 |
|       |             | MSE      | 0.0648  | 0.0698   | 0.0680 |
| B     | 200         | Bias     | -0.0136 | 0.0463   | 0.0356 |
|       |             | Var      | 0.0261  | 0.0275   | 0.0272 |
|       |             | MSE      | 0.0263  | 0.0296   | 0.0285 |
|       | 500         | Bias     | -0.0122 | 0.0426   | 0.0313 |
|       |             | Var      | 0.0121  | 0.0129   | 0.0129 |
|       |             | MSE      | 0.0123  | 0.0147   | 0.0139 |
|       | 1000        | Bias     | -0.0223 | 0.0384   | 0.0283 |
|       |             | Var      | 0.0748  | 0.0811   | 0.0792 |
|       |             | MSE      | 0.0753  | 0.0825   | 0.0800 |
| C     | 200         | Bias     | -0.0141 | 0.0369   | 0.0287 |
|       |             | Var      | 0.0281  | 0.0307   | 0.0301 |
|       |             | MSE      | 0.0283  | 0.0320   | 0.0309 |
|       | 500         | Bias     | -0.0142 | 0.0310   | 0.0221 |
|       |             | Var      | 0.0124  | 0.0138   | 0.0136 |
|       |             | MSE      | 0.0126  | 0.0148   | 0.0141 |
The simulation results in Table 1 shows that the three methods show similar results under the linear model (Model A), but kernel ridge regression imputation shows the best performance in terms of the mean square errors under the nonlinear models (Models B and C). Linear regression imputation still provides unbiased estimates, because the residual terms in the linear regression model are approximately unbiased to zero. However, use of linear regression model for imputation leads to efficiency loss because it is not the best model.

In addition, we have computed the proposed variance estimator under kernel ridge regression imputation. In Table 2 the relative biases of the proposed variance estimator and the coverage rates of two interval estimators under 90% and 95% nominal coverage rates are presented. The relative bias of the variance estimator decreases as the sample size increases, which confirms the validity of the proposed variance estimator. Furthermore, the interval estimators show good performances in terms of the coverage rates.

Table 2: Relative biases (R.B.) of the proposed variance estimator, coverage rates (C.R.) of the 90% and 95% confidence intervals for imputed estimators under kernel ridge regression imputation for continuous responses

| Model | Criteria     | Sample Size |
|-------|--------------|-------------|
|       |              | 200  | 500  | 1000 |
| A     | R.B.         | -0.105 | -0.064 | -0.031 | 87.5% | 89.6% | 89.9% |
|       | C.R. (90%)   | 94.0%  | 94.7% | 94.9% | 87.6% | 87.0% | 89.2% |
|       | C.R. (95%)   |        |       |       | 92.6% | 93.3% | 94.8% |
| B     | R.B.         | -0.101 | -0.108 | -0.028 | 85.0% | 86.2% | 90.4% |
|       | C.R. (90%)   | 91.4%  | 93.4% | 94.6% | 91.4% | 93.4% | 94.6% |
4.2 Simulation study two

The second simulation study is similar to the first simulation study except that the study variable $Y$ is binary. We use the same simulation setup for generating $x_i = (x_{1i}, x_{2i}, x_{3i}, x_{4i})$ and $\delta_i$ as the first simulation study. We consider three models for generating $Y$

$$y_i \sim \text{Bernoulli}(p_i),$$

where $p_i$ is chosen differently for each model. For model D, we have

$$\text{logit}(p_i) = 0.5 + (1/35)x_{i2}^2 x_{i3}^3 + 0.1x_{i4}.$$  

The responses for Model E are generated by (18) with

$$\text{logit}(p_i) = 0.5 + (1/180)x_{i1}^2 x_{i2} x_{i3}^2 x_{i4}^2.$$  

The responses for Model F are generated by (18) with

$$\text{logit}(p_i) = 0.5 + 0.15x_{i1} x_{i2} x_{i3}^2 + 0.4x_{i2} x_{i3}.$$  

For each model, we consider three imputation estimators: kernel ridge regression (KRR), B-spline, linear regression (Linear). We compute the Monte Carlo biases, variance, and the mean squared errors of the imputation estimators for each case. The comparison of the simulation results for different estimators are presented in Table 3. In addition, the relative biases and the coverage rates of the interval estimators are presented in Table 4. The simulation results in Table 4 show that the relative biases of the variance estimators are negligible and the coverage rates of the interval estimators are close to the nominal levels.
Table 3: Biases, Variances and Mean Squared Errors (MSEs) of three imputation estimators for binary responses

| Model | Sample Size | Criterion | KRR   | B-spline | Linear |
|-------|-------------|-----------|-------|----------|--------|
|       |             | Bias      | 0.00028 | 0.00007  | 0.00009 |
|       |             | Var       | 0.00199 | 0.00208  | 0.00206 |
|       |             | MSE       | 0.00199 | 0.00208  | 0.00206 |
| D     | 200         | Bias      | -0.00019 | -0.00014 | -0.00019 |
|       |             | Var       | 0.00080  | 0.00081  | 0.00081 |
|       |             | MSE       | 0.00080  | 0.00081  | 0.00081 |
|       | 500         | Bias      | -0.00006 | -0.00010 | -0.00010 |
|       |             | Var       | 0.00042  | 0.00042  | 0.00042 |
|       | 1000        | Bias      | 0.00027  | -0.00001 | -0.00003 |
|       |             | Var       | 0.00195  | 0.00204  | 0.00202 |
|       |             | MSE       | 0.00195  | 0.00204  | 0.00202 |
| E     | 200         | Bias      | -0.00039 | -0.00042 | -0.00044 |
|       |             | Var       | 0.00079  | 0.00080  | 0.00080 |
|       |             | MSE       | 0.00079  | 0.00080  | 0.00080 |
|       | 500         | Bias      | -0.00005 | -0.00013 | -0.00010 |
|       |             | Var       | 0.00042  | 0.00043  | 0.00043 |
|       |             | MSE       | 0.00042  | 0.00043  | 0.00043 |
|       | 1000        | Bias      | 0.00077  | 0.00102  | 0.00100 |
|       |             | Var       | 0.00199  | 0.00208  | 0.00206 |
|       |             | MSE       | 0.00199  | 0.00208  | 0.00206 |
| F     | 200         | Bias      | -0.00002 | 0.00054  | 0.00047 |
|       |             | Var       | 0.00079  | 0.00080  | 0.00080 |
|       |             | MSE       | 0.00079  | 0.00080  | 0.00080 |
|       | 500         | Bias      | 0.00007  | 0.00055  | 0.00060 |
|       |             | Var       | 0.00042  | 0.00043  | 0.00043 |
|       |             | MSE       | 0.00042  | 0.00043  | 0.00043 |
|       | 1000        | Bias      | 0.00007  | 0.00055  | 0.00060 |
|       |             | Var       | 0.00042  | 0.00043  | 0.00043 |
|       |             | MSE       | 0.00042  | 0.00043  | 0.00043 |

5 Application

We applied the KRR with kernels of second-order Sobolev space and Gaussian kernel to study the PM$_{2.5}(\mu g/m^3)$ concentration measured in Beijing, China (Liang et al., 2015). Hourly weather conditions: temperature, air pressure,
Table 4: Relative biases (R.B.) of the proposed variance estimator, coverage rates (C.R.) of the 90% and 95% confidence intervals for imputed estimators under kernel ridge regression imputation for binary responses

| Model | Criteria                  | Sample Size |
|-------|---------------------------|-------------|
|       |                           | 200  | 500  | 1000 |
| D     | R.B.                      | -0.0061 | 0.0068 | -0.0392 |
|       | C.R. (90%)                | 88.6% | 90.2% | 90.4% |
|       | C.R. (95%)                | 94.6% | 94.1% | 94.3% |
| E     | R.B.                      | 0.0165 | 0.0222 | -0.0487 |
|       | C.R. (90%)                | 89.2% | 89.9% | 89.6% |
|       | C.R. (95%)                | 94.6% | 94.7% | 93.9% |
| F     | R.B.                      | -0.0062 | 0.0187 | -0.0437 |
|       | C.R. (90%)                | 89.9% | 89.7% | 89.9% |
|       | C.R. (95%)                | 94.7% | 94.8% | 94.3% |

Cumulative wind speed, cumulative hours of snow and cumulative hours of rain are available from 2011 to 2015. Meanwhile, the averaged sensor response is subject to missingness. In December 2012, the missing rate of PM$_{2.5}$ is relatively high with missing rate 17.47%. We are interested in estimating the mean PM$_{2.5}$ in December with imputed KRR estimates. The point estimates and their 95% confidence intervals are presented in the Table 5. The corresponding results are presented in the Figure 5. As a benchmark, the confidence interval computed from complete cases (Complete in Table 5) and confidence intervals for the imputed estimator under linear model (Linear) (Kim and Rao, 2009) are also presented there.

As we can see, the performances of KRR imputation estimators are similar and created narrower 95% confidence intervals. Furthermore, the imputed PM$_{2.5}$ concentration during the missing period is relatively lower than the fully observed weather conditions on average. Therefore, if we only utilize the complete cases to estimate the mean of PM$_{2.5}$, the severeness of air pollution would be over-estimated.
Table 5: Imputed estimates (I.E.), standard error (S.E.) and 95% confidence intervals (C.I.) for imputed mean PM$_{2.5}$ in December, 2012 under kernel ridge regression

| Estimator | I.E. | S.E.  | 95% C.I.     |
|-----------|-----|------|--------------|
| Complete  | 109.20 | 3.91 | (101.53, 116.87) |
| Linear    | 99.61  | 3.68 | (92.39, 106.83) |
| Sobolev   | 102.25 | 3.50 | (95.39, 109.12) |
| Gaussian  | 101.30 | 3.53 | (94.37, 108.22) |

Figure 1: Estimated mean PM$_{2.5}$ concentration in December 2012 with 95% confidence interval.

6 Discussion

We consider kernel ridge regression as a tool for nonparametric imputation and establish its asymptotic properties. In addition, we propose a linearized approach for variance estimation of the imputed estimator. For variance estimation, we also propose a novel approach of the maximum entropy method for propensity score estimation. The proposed Kernel ridge regression imputation can be used as a general tool for nonparametric imputation. By choosing different kernel functions, different nonparametric imputation methods can be developed. The unified theory developed in this paper can cover various types of the kernel ridge regression.
imputation and enables us to make valid statistical inferences about the population means.

There are several possible extensions of the research. First, the theory can be directly applicable to other nonparametric imputation methods, such as smoothing splines (Claeskens et al., 2009). Second, instead of using ridge-type penalty term, one can also consider other penalty functions such as SCAD penalty (Fan and Li, 2001) or adaptive Lasso (Zou, 2006). Also, the maximum entropy method for propensity score estimation should be investigated more rigorously. Such extensions will be future research topics.

Appendix

A. Proof of Theorem 1

Before we prove the main theorem, we first introduce the following lemma.

Lemma 2 (modified Lemma 7 in Zhang et al. (2013)). Suppose Assumption [A1] and [A2] hold, for a random vector \( z = \mathbb{E}(z) + \sigma \varepsilon \), let \( \bar{\lambda} = \lambda/n \) we have

\[
S_{\lambda} z = \mathbb{E}(z \mid x) + O_p \left( \bar{\lambda} + \sqrt{\frac{\gamma(\bar{\lambda})}{n}} \right) 1_n,
\]

as long as \( \mathbb{E}(\|z_i\|_H) \) and \( \sigma^2 \) is bounded from above, for \( i = 1, \ldots, n \), where \( \varepsilon \) are noise vector with mean zero and bounded variance and

\[
\gamma(\bar{\lambda}) := \sum_{j=1}^{\infty} \frac{1}{1 + \bar{\lambda}/\mu_j},
\]

is the effective dimension and \( \{\mu_j\}_{j=1}^{\infty} \) are the eigenvalues of kernel \( K \) used in \( \hat{m}(x) \).
Now, to prove our main theorem, we write

\[
\hat{\theta}_I = \frac{1}{n} \sum_{i=1}^{n} \{ \delta_i y_i + (1 - \delta_i) \hat{m}(x_i) \}
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} m(x_i) + \frac{1}{n} \sum_{i=1}^{n} \delta_i \{ y_i - m(x_i) \} + \frac{1}{n} \sum_{i=1}^{n} (1 - \delta_i) \{ \hat{m}(x_i) - m(x_i) \}.
\]

\(\boxed{R_n \leq \sum_{i=1}^{n} \delta_i \{ y_i - m(x_i) \} + o_p(n^{-1/2}),}

(A.1)

Therefore, as long as we show

\[
T_n = \frac{1}{n} \sum_{i=1}^{n} \delta_i \left\{ \frac{1}{\pi(x_i)} - 1 \right\} \{ y_i - m(x_i) \} + o_p(n^{-1/2}),
\]

(A.2)

then the main theorem automatically holds.

To show (A.2), recall that the KRR can be regarded as the following optimization problem

\[
\hat{\alpha}_\lambda = \arg \min_{\alpha \in \mathbb{R}^n} (y - K\alpha)^T \Delta_n (y - K\alpha) + \lambda \alpha^T K\alpha.
\]

Further, we have

\[
\hat{\alpha}_\lambda = (\Delta_n K + \lambda I_n)^{-1} \Delta_n y,
\]

and

\[
\hat{m} = K (\Delta_n K + \lambda I_n)^{-1} \Delta_n y
\]

\[
= K \left\{ (\Delta_n + \lambda K^{-1}) K \right\}^{-1} \Delta_n y
\]

\[
= (\Delta_n + \lambda K^{-1})^{-1} \Delta_n y,
\]

where \(\hat{m} = (\hat{m}(x_1), \ldots, \hat{m}(x_n))^T\). Let \(S_\lambda = (I_n + \lambda K^{-1})^{-1}\), we have

\[
\hat{m} = (\Delta_n + \lambda K^{-1})^{-1} \Delta_n y = C_n^{-1} d_n,
\]

19
where

\[ C_n = S_\lambda \left( \Delta_n + \lambda K^{-1} \right), \]
\[ d_n = S_\lambda \Delta_n y. \]

By Lemma 2 let \( \tilde{\lambda} = \lambda/n \), we obtain

\[ C_n = \mathbb{E}(\Delta_n \mid x) + O_p \left( \tilde{\lambda} + \sqrt{\frac{\gamma(\tilde{\lambda})}{n}} \right) 1_n \]
\[ := \Pi + O_p \left( \tilde{\lambda} + \sqrt{\frac{\gamma(\tilde{\lambda})}{n}} \right) 1_n, \]

where \( \Pi = \text{diag}(\pi(x_1), \ldots, \pi(x_n)) \) and \( \gamma(\tilde{\lambda}) \) is the effective dimension of kernel \( K \). Similarly, we have

\[ d_n = \mathbb{E}(\Delta_n y \mid x) + O_p \left( \tilde{\lambda} + \sqrt{\frac{\gamma(\tilde{\lambda})}{n}} \right) 1_n \]
\[ = \Pi m + O_p \left( \tilde{\lambda} + \sqrt{\frac{\gamma(\tilde{\lambda})}{n}} \right) 1_n. \]

Consequently, letting \( a_n = \tilde{\lambda} + \sqrt{\frac{\gamma(\tilde{\lambda})}{n}} \) and applying Taylor expansion, we have

\[ \hat{m} = m + \Pi^{-1} (d_n - C_n m) + o_p(a_n) 1_n \]
\[ = m + \Pi^{-1} \left( S_\lambda \Delta_n y - S_\lambda \left( \Delta_n + \lambda K^{-1} \right) m \right) \]
\[ + o_p(a_n) 1_n \]
\[ = m + \Pi^{-1} S_\lambda \Delta_n (y - m) + O_p(a_n) 1_n, \]

20
where the last equality holds because
\[
S_\lambda K^{-1} m = S_\lambda \left\{ (I_n + \lambda K^{-1}) - I_n \right\} m
= m - S_\lambda m = O_p(a_n).
\]

Therefore, we have
\[
T_n = n^{-1} 1^T (I_n - \Delta_n) (\hat{m} - m)
= n^{-1} 1^T (I_n - \Delta_n) \Pi^{-1} S_\lambda \Delta_n (y - m) + O_p(a_n)
= n^{-1} 1^T (I_n - \Pi) \Pi^{-1} \Delta_n (y - m) + O_p(a_n)
= n^{-1} 1^T \left( \Pi^{-1} - I_n \right) \Delta_n (y - m) + O_p(a_n).
\]

By Corollary 5 in [Zhang et al., 2013], for \(\ell\)-th order of Sobolev space, we have
\[
\gamma(\tilde{\lambda}) = \sum_{j=1}^{\infty} \frac{1}{1 + j^{2\ell}}
\leq \tilde{\lambda}^{-\frac{1}{2\ell}} + \sum_{j>\tilde{\lambda}^{-\frac{1}{2\ell}}}^{\infty} \frac{1}{1 + j^{2\ell}}
\leq \tilde{\lambda}^{-\frac{1}{2\ell}} + \tilde{\lambda}^{-1} \int_{\tilde{\lambda}^{-\frac{1}{2\ell}}}^{\infty} z dz
= \tilde{\lambda}^{-\frac{1}{2\ell}} + \frac{1}{2\ell - 1} \tilde{\lambda}^{-\frac{1}{2\ell}}
= O \left( \tilde{\lambda}^{-\frac{1}{2\ell}} \right).
\] (A.3)

Consequently, as long as \(\tilde{\lambda}^{-\frac{1}{2\ell}}/n = o(1)\) and \(\tilde{\lambda} = o(n^{-1/2})\), we have
\[
T_n = \frac{1}{n} 1^T \left( \Pi^{-1} - I_n \right) \Delta_n (y - m) + o_p(n^{-1/2}).
\] (A.4)

One legitimate of such \(\tilde{\lambda}\) can be chosen as \(n^{-\ell}\), i.e., \(\lambda = O(n^{1-\ell})\).
B. Computational Details

As the objective function in (13) is convex (Nguyen et al., 2010), we apply the limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) algorithm to solve the optimization problem with the following first order partial derivatives:

\[
\frac{\partial U}{\partial \alpha_0} = \frac{1}{n_1} \sum_{i=1}^{n} \mathbb{I}(\delta_i = 0) \exp \left( \alpha_0 + \sum_{j=1}^{n} \alpha_j K(x_i, x_j) \right) - 1,
\]

\[
\frac{\partial U}{\partial \alpha_k} = \frac{1}{n_1} \sum_{i=1}^{n} \mathbb{I}(\delta_i = 0) K(x_i, x_k) \exp \left( \alpha_0 + \sum_{j=1}^{n} \alpha_j K(x_i, x_j) \right) - \frac{1}{n_0} \sum_{i=1}^{n} K(x_i, x_k)
\]

\[+ 2\tau \sum_{i=1}^{n} K(x_i, x_k) \alpha_i, k = 1, \ldots, n.\]

For tuning parameter selection \(\tau\) in (12), we adopt a cross-validation (CV) strategy. In particular, we may firstly stratify the sample \(S = \{1, \ldots, n\}\) into two strata \(S_0 = \{i \in S : \delta_i = 0\}\) and \(S_1 = \{i \in S : \delta_i = 1\}\). Within each \(S_h\), we make \(K\) random partition \(A_k^{(h)}\) such that

\[\bigcup_{k=1}^{K} A_k^{(h)} = S_h, h = 0, 1\]

\[A_{k_1}^{(h)} \bigcap A_{k_2}^{(h)} = \emptyset, k_1 \neq k_2, k_1, k_2 \in \{1, \ldots, K\},\]

\[|A_1^{(h)}| \approx |A_2^{(h)}| \approx \cdots \approx |A_K^{(h)}|, h = 0, 1,\]

where \(|\cdot|\) is the cardinality of a specific set. For a fixed \(\tau > 0\), the corresponding CV criterion is

\[
\text{CV}(\tau) = \frac{1}{K} \sum_{k=1}^{K} \sum_{j \in A_k} \hat{L}(\delta_j, \hat{g}^{(-k)}(x_j, \tau)),
\]

(A.5)

where \(\hat{g}^{(-k)}\) is the trained model with data with data points except for \(A_k = A_k^{(0)} \cup A_k^{(1)}\). Regarding the loss function in (A.5), we can use

\[
\hat{L}(\delta; \hat{g}) = \mathbb{I}(\delta = 1, \hat{p}(x) < 0.5) + \mathbb{I}(\delta = 0, \hat{p}(x) > 0.5),
\]

22
where \( \hat{p}(x) = n_1 / \{n_1 + n_0 \hat{g}(x)\} \) as an estimator for \( p(x) = Pr(\delta = 1 \mid x) \). As a result, we may select the tuning parameter \( \tau \) which minimizes the CV criteria in (A.5).

**References**

Aronszajn, N. (1950). Theory of reproducing kernels. *Transactions of the American mathematical society* 68(3), 337–404.

Cheng, P. E. (1994). Nonparametric estimation of mean functionals with data missing at random. *J. Am. Statist. Assoc.* 89(425), 81–87.

Claeskens, G., T. Krivobokova, and J. D. Opsomer (2009). Asymptotic properties of penalized spline estimators. *Biometrika* 96, 529–544.

Fan, J. and R. Li (2001). Variable selection via nonconcave penalized likelihood and its Oracle properties. *J. Am. Statist. Assoc.* 96, 1348–1360.

Friedman, J., T. Hastie, and R. Tibshirani (2001). *The elements of statistical learning*, Volume 1. Springer series in statistics New York.

Haziza, D. (2009). Imputation and inference in the presence of missing data. In *Handbook of statistics*, Volume 29, pp. 215–246. Elsevier.

Kalton, G. and L. Kish (1984). Some efficient random imputation methods. 13(16), 1919–1939.

Kim, J. K. (2011). Parametric fractional imputation for missing data analysis. *Biometrika* 98(1), 119–132.
Kim, J. K., J. Michael Brick, W. A. Fuller, and G. Kalton (2006). On the bias of the multiple-imputation variance estimator in survey sampling. *J. R. Statist. Soc. B* 68(3), 509–521.

Kim, J. K. and J. Rao (2009). A unified approach to linearization variance estimation from survey data after imputation for item nonresponse. *Biometrika* 96(4), 917–932.

Kim, J. K. and J. Shao (2013). *Statistical methods for handling incomplete data*. CRC press.

Kim, J. K. and S. Yang (2014). Fractional hot deck imputation for robust inference under item nonresponse in survey sampling. *Survey Methodol.* 40(2), 211.

Koltchinskii, V. et al. (2006). Local rademacher complexities and oracle inequalities in risk minimization. *Ann. Statist.* 34(6), 2593–2656.

Liang, X., T. Zou, B. Guo, S. Li, H. Zhang, S. Zhang, H. Huang, and S. X. Chen (2015). Assessing beijing’s pm2.5 pollution: severity, weather impact, apec and winter heating. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* 471(2182), 20150257.

Little, R. J. and D. B. Rubin (2019). *Statistical analysis with missing data*, Volume 793. John Wiley & Sons.

Mendelson, S. (2002). Geometric parameters of kernel machines. In *International Conference on Computational Learning Theory*, pp. 29–43. Springer.

Nguyen, X., M. J. Wainwright, and M. I. Jordan (2010). Estimating divergence
functionals and the likelihood ratio by convex risk minimization. *IEEE Transactions on Information Theory* 56(11), 5847–5861.

Owen, A. B. (2001). *Empirical likelihood*. CRC press.

Qin, J. and J. Lawless (1994). Empirical likelihood and general estimating equations. *Ann. Statist.*, 300–325.

Robins, J. M., A. Rotnitzky, and L. P. Zhao (1994). Estimation of regression coefficients when some regressors are not always observed. *J. Am. Statist. Assoc.* 89, 846–866.

Rubin, D. B. (1976). Inference and missing data. *Biometrika* 63(3), 581–592.

Rubin, D. B. (2004). *Multiple imputation for nonresponse in surveys*, Volume 81. John Wiley & Sons.

Shawe-Taylor, J., N. Cristianini, et al. (2004). *Kernel methods for pattern analysis*. Cambridge university press.

Steinwart, I., D. R. Hush, C. Scovel, et al. (2009). Optimal rates for regularized least squares regression. In *COLT*, pp. 79–93.

van de Geer, S. A. (2000). *Empirical Processes in M-estimation*, Volume 6. Cambridge university press.

Wahba, G. (1990). *Spline models for observational data*, Volume 59. Siam.

Wang, D. and S. X. Chen (2009). Empirical likelihood for estimating equations with missing values. *Ann. Statist.* 37(1), 490–517.
Wang, N. and J. M. Robins (1998). Large-sample theory for parametric multiple imputation procedures. *Biometrika* 85(4), 935–948.

Yang, S. and J. Kim (2016). A note on multiple imputation for general-purpose estimation. *Biometrika* 103, 244–251.

Zhang, T. (2005). Learning bounds for kernel regression using effective data dimensionality. *Neural Computation* 17(9), 2077–2098.

Zhang, Y., J. Duchi, and M. Wainwright (2013). Divide and conquer kernel ridge regression. In *Conference on learning theory*, pp. 592–617.

Zou, H. (2006). The adaptive Lasso and its oracle properties. *J. Am. Statist. Assoc.* 101, 1418–1429.