

A note on model selection for small sample regression

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Abstract The risk estimator called “Direct Eigenvalue Estimator” (DEE) is studied. DEE was developed for small sample regression. In contrast to many existing model selection criteria, derivation of DEE requires neither any asymptotic assumption nor any prior knowledge about the noise variance and the noise distribution. It was reported that DEE performed well in small sample cases but DEE performed a little worse than the state-of-the-art ADJ. This seems somewhat counter-intuitive because DEE was developed for specifically regression problem by exploiting available information exhaustively, while ADJ was developed for general setting. In this paper, we point out that the derivation of DEE includes an inappropriate part, notwithstanding the resultant form of DEE being valid in a sense. As its result, DEE cannot derive its potential. We introduce a class of ‘valid’ risk estimators based on the idea of DEE and show that better risk estimators (mDEE) can be found in the class. By numerical experiments, we verify that mDEE often performs better than or at least equally the original DEE and ADJ.

Keywords Finite sample · Regression · Model selection · Unlabeled data

1 Introduction

The most famous approach of model selection is to derive a risk estimator and to choose the model minimizing it. This type of model selection includes cross-validation and so-called “information criteria” including AIC (Akaike 1973), BIC (Schwartz 1979), GIC (Konishi

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and Kitagawa 1996) and so on. Basically, information criteria have been derived by using asymptotic expansion, which requires the sample number n to go to the infinity. Though the cross-validation was not derived by asymptotic assumption, its unbiasedness or performance is guaranteed basically by asymptotic theory. For regression, Chapelle et al. (2002) proposed an interesting model selection criteria called Direct Eigenvalue Estimator (DEE). DEE has the following remarkable characteristics: (i) DEE is an approximately unbiased risk estimator for finite n . (ii) no asymptotic assumption ($n \rightarrow \infty$) is necessary to derive it. (iii) no prior knowledge about the noise variance and the noise distribution is necessary. Due to these virtues, DEE is expected to perform nicely for small sample cases. DEE requires two assumptions in its derivation instead of using the asymptotic assumption. The first assumption is that a large number of unlabeled data are available in addition to the labeled data. This assumption is often made in recent machine learning literatures and is practical because the unlabeled data can usually be gathered automatically. The other assumption is the most important assumption, which imposes statistical independence between the inside-the-model part and the outside-the-model part of the dependent variable y . This assumption holds not exactly in general but hold approximately. By numerical experiments, Chapelle et al. (2002) showed that DEE performed better than many of the conventional information criteria and the cross-validation. However, they also reported that another criterion ADJ (Schuurmans 1997) often performed better than DEE. It should be noted here that the comparison between ADJ and DEE is fair since ADJ also assumes that a lot of unlabeled data are available. Even though ADJ is the state-of-the-art, that result seems somewhat strange because DEE was derived specifically for regression by exploiting the properties of regression exhaustively while the derivation of ADJ is somewhat heuristic and was developed for general setting. By careful investigation, we found an inappropriate part in the derivation process of DEE, although the resultant form of DEE is ‘valid’ in a sense. As a result, DEE cannot derive its potential. To clarify these facts, we formulate the derivation process of DEE again and introduce a class of ‘valid’ risk estimators based on the idea of DEE. Then, we show that DEE belongs to this class but is not close to the optimal estimator among this class. Indeed, we can find several more reasonable risk estimators (mDEE) in this class. The variations arise from how to balance a certain bias-variance trade-off. The performance of mDEE is investigated by numerical experiments. We compare the performance of mDEE with the original DEE, ADJ and other existing model selection methods.

This paper is an extended version of the conference paper (Kawakita et al. 2010). We pointed out the above inappropriate part in the derivation of DEE and proposed a naive modification in the paper. However, theoretical analysis and numerical experiments are significantly strengthened in this paper.

The paper is organized as follows. We set up a regression problem and introduce some notations in Sect. 2. In Sect. 3, we briefly review the result of Chapelle et al. (2002) and explain which part is inappropriate in the derivation of DEE. In Sect. 4, a class of valid risk estimators are defined. We explain why DEE is valid but not close to the optimal estimator in this class. In addition, some modifications of DEE are proposed. All of proofs of our theorems are given in Sect. 5. Section 6 provided numerical experiments to investigate the performance of our proposal. The conclusion is described in Sect. 7.

2 Setup and notations

We employ a usual regression setting as reviewed briefly below. Let $\mathcal{X} \subset \mathfrak{R}^M$ and $\mathcal{Y} := \mathfrak{R}$. Suppose that we have training data $D := \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$ generated from the

joint density $p(x, y) = p(x)p(y|x)$ i.i.d. (independently and identically distributed), where $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$ for each i . Here, we further assume the following regression model:

$$y_i = f_*(x_i) + \xi_i, \tag{1}$$

where $f_*(x)$ is a certain regression function belonging to $L^2(\mathcal{X})$ and ξ_i is a noise random variable which is subject to $p_\xi(\xi)$ with mean zero and variance σ^2 and is independent of x . This implies that $p(y|x) = p_\xi(y - f_*(x))$. The goal of regression problem is to estimate $f_*(x)$ based on the given data set. To estimate $f_*(x)$, let us consider a model of regression function defined by

$$f(x; \bar{\alpha}) := \sum_{k=1}^{\infty} \bar{\alpha}_k \phi_k(x), \tag{2}$$

where $\bar{\alpha} = (\bar{\alpha}_1, \bar{\alpha}_2, \dots)^T$. Here, T denotes the transposition of vectors or a matrices. Just for convenience, we can assume that $\{\phi_k(x)\}$ is a basis of $L_2(\mathcal{X})$. If not, we can always extend it as such without loss of generality. By this assumption, there exists $\bar{\alpha}^* := (\bar{\alpha}_1^*, \bar{\alpha}_2^*, \dots)^T$ such that $f_*(x) \equiv f(x; \bar{\alpha}^*)$ almost everywhere. Our task now reduces to find an estimator $\hat{f}(x)$ of $f(x; \bar{\alpha}^*)$ as accurate as possible. Its accuracy is measured by the loss function (Mean Squared Error) defined as

$$L(\hat{f}) := E_{x,y} \left[(y - \hat{f}(x))^2 \right]. \tag{3}$$

Here, $E_{x,y}[\cdot]$ denotes the expectation with respect to random variables x, y . Similarly, each expectation E has subscripts expressing over which random variables the expectation is taken. Since $f(x; \bar{\alpha})$ essentially can express an arbitrary element of $L^2(\mathcal{X})$, $f(x; \bar{\alpha})$ itself is too flexible and tends to cause overfitting in general. Therefore, we usually use a truncated version of $f(x; \bar{\alpha})$ as a model

$$\mathcal{M}_d := \left\{ f_d(x; \alpha) := \sum_{k=1}^d \alpha_k \phi_k(x) \mid \alpha = (\alpha_1, \alpha_2, \dots, \alpha_d)^T \in \mathbb{R}^d \right\},$$

where d is a positive integer. The ideal estimate of parameter α is obtained by minimizing the loss function L in (3) with respect to α . However, L is not available because the distribution $p(x, y)$ is unknown. Therefore, we usually minimize an empirical loss function based on D , which is defined as

$$L_D(f_d(\cdot; \alpha)) := \frac{1}{n} \sum_{i=1}^n (y_i - f_d(x_i; \alpha))^2. \tag{4}$$

For notation simplicity, we define $y = (y_1, y_2, \dots, y_n)^T$ and Φ as $(n \times d)$ matrix whose (i, k) component is $\phi_k(x_i)$. Then, $L_D(f_d(\cdot; \alpha)) = (1/n) \|y - \Phi\alpha\|^2$, where $\|\cdot\|$ is the Euclidean norm. The estimator $\hat{\alpha}(D)$ minimizing L_D is referred to as Least Squares Estimator (LSE), i.e.,

$$\hat{\alpha}(D) := \operatorname{argmin}_{\alpha \in \mathbb{R}^d} L_D(f_d(\cdot; \alpha)) = (\Phi^T \Phi)^{-1} \Phi^T y. \tag{5}$$

We sometimes drop (D) of $\hat{\alpha}(D)$ for notation simplicity. An important task is to choose the optimal d . When d is too large, f_d tends to overfit, while f_d cannot approximate $f_*(x)$ with too small d . To choose d , we assume that additional unlabeled data $D_U := \{x'_1, x'_2, \dots, x'_n\}$ are available, where each x'_j is subject to $p(x)$ independently. The number of unlabeled

data n' is assumed to be significantly larger than n . Note that D_U is used not for parameter estimation but only for model selection as well as [Chapelle et al. \(2002\)](#). The basic idea to choose d is as follows. The following risk (expected loss function)

$$R^*(d) := E_D[L(f_d(\cdot; \hat{\alpha}(D)))] \tag{6}$$

is often employed to measure the performance of the model. Hence, one of natural strategies is deriving an estimate of $R^*(d)$ (denoted by $\hat{R}_D(d)$) using $D \cup D_U$, and then choosing the model as $\hat{d} := \operatorname{argmin}_d \hat{R}_D(d)$. Many researchers have proposed estimators of $R^*(d)$ so far. In the next section, we introduce one of such estimators, which was proposed by [Chapelle et al. \(2002\)](#).

3 Review of direct eigenvalue estimator

Most of past information criteria have been derived based on asymptotic expansion. That is, they postulate that $n \rightarrow \infty$. In contrast, [Chapelle et al. \(2002\)](#) derived a risk estimator called DEE (Direct Eigenvalue Estimator) without using asymptotic assumption. In this section, we briefly review DEE and explain that its derivation includes an inappropriate part. As is well known, $L_D(f_d(\cdot; \hat{\alpha}(D)))$ is not an unbiased estimator of $R^*(d)$. That is,

$$\operatorname{bias}(L_D(f_d(\cdot; \hat{\alpha}(D)))) := E_D[L_D(f_d(\cdot; \hat{\alpha}(D)))] - R^*(d)$$

is not equal to zero. Let $T^*(n, d)$ be

$$T^*(n, d) = \frac{E_D[L(f_d(\cdot; \hat{\alpha}(D)))]}{E_D[L_D(f_d(\cdot; \hat{\alpha}(D)))]}.$$

Using $T^*(n, d)$, let us consider the following risk estimator

$$\hat{R}_D^*(d) := T^*(n, d)L_D(f_d(\cdot; \hat{\alpha}(D))).$$

It is immediate to see that this estimator is exactly unbiased, i.e., $\operatorname{bias}(\hat{R}_D^*(d)) = 0$. That is, $T^*(n, d)$ is a so-called bias-correcting term. Remarkably, this estimator corrects the bias multiplicatively, whereas the most of existing information criteria correct the bias additively like AIC. [Chapelle et al. \(2002\)](#) showed that $T^*(n, d)$ can be calculated as the following theorem.

Theorem 1 ([Chapelle et al. 2002](#)) *Let $\phi_1(x) \equiv 1$. Define $\hat{C} := (1/n)\Phi^T \Phi$. Suppose that the following assumptions hold.*

A1 *Assume that $\{\phi_k(x) | k = 1, 2, \dots, d\}$ is orthonormal with respect to the expectation inner product $\langle a(x), b(x) \rangle_p := E_x[a(x)b(x)]$, i.e.,*

$$\forall k, \forall k', \quad \langle \phi_k(X), \phi_{k'}(X) \rangle_p = \delta_{kk'}, \tag{7}$$

where $\delta_{kk'}$ is Kronecker's delta.

A2 *Let $f_d^* := \min_{f \in \mathcal{M}_d} L(f)$. Define $\tilde{y}_i := y_i - f_d^*(x_i)$ and $\tilde{y} := (\tilde{y}_1, \tilde{y}_2, \dots, \tilde{y}_n)^T$. Assume that*

$$\text{“}\tilde{y} \text{ and } \Phi \text{ are statistically independent.”} \tag{8}$$

Then $T^*(n, d)$ is exactly calculated as

$$T^*(n, d) = \frac{1 + (1/n)E_D[\operatorname{Tr}(\hat{C}^{-1})]}{1 - (d/n)}. \tag{9}$$

See [Chapelle et al. \(2002\)](#) for the meaning of the assumption A2. A key fact is that Theorem 1 holds for finite n and the resultant form of $T^*(n, d)$ does not depend on any unknown quantities except $E_D[\text{Tr}(\widehat{C}^{-1})]$. In addition, it seems to be not difficult to find valid estimators of $E_D[\text{Tr}(\widehat{C}^{-1})]$. Indeed, [Chapelle et al. \(2002\)](#) derived its estimator as

$$\text{Tr}(\widehat{C}^{-1}\widetilde{C}), \tag{10}$$

where \widetilde{C} is defined by $\widetilde{C} = \frac{1}{n'}(\Phi')^T \Phi'$ and Φ' is an $(n' \times d)$ matrix whose (j, k) component is $\phi_k(x'_j)$. The resultant risk estimator is called DEE and is given by

$$\widehat{R}_D^{\text{DEE}}(d) = \frac{1 + (1/n)\text{Tr}(\widehat{C}^{-1}\widetilde{C})}{1 - (d/n)} L_D(f_d(\cdot; \hat{\alpha}(D))). \tag{11}$$

Note that the resultant bias correction factor is invariant under coordinate transformation. That is, the orthonormal assumption (7) can be removed by chance. However, this is somewhat queer. DEE was derived based on (9) but (9) is not invariant under coordinate transformation (it was derived by assuming the orthonormality of basis). Actually, (10) is not a consistent estimator of $E_D[\text{Tr}(\widehat{C}^{-1})]$ in non-orthonormal case. This is because the derivation of estimator (10) includes an inappropriate part. We explain it in the remark at the end of this section. However, we must emphasize that the resultant form of DEE in (11) is valid as a risk estimator in a sense in spite of the above fact. Indeed, DEE dominated other model selection methods in numerical experiments, as reported by [Chapelle et al. \(2002\)](#). However, due to the inappropriate derivation, DEE cannot demonstrate its potential performance. We will explain it in details in the next section.

Remark We explain here which part of the derivation of DEE is inappropriate. [Chapelle et al. \(2002\)](#) derived (10) as follows. First, they rewrote $E_D[\text{Tr}(\widehat{C}^{-1})]$ as

$$E_D[\text{Tr}(\widehat{C}^{-1})] = E_D \left[\sum_{k=1}^d (1/\lambda_k) \right],$$

where λ_k is the k -th eigenvalue of \widehat{C} . The subsequent part is described by quoting the corresponding part of their paper (page 16 of [Chapelle et al. \(2002\)](#)). Note that some notations and equation numbers are replaced in order to be consistent with this paper.

Quote 1 (Derivation of DEE) *In the case when along with training data, unlabeled data are available (x without y), one can compute two covariance matrices: one from unlabeled data \widetilde{C} and another from the training data \widehat{C} . There is a unique matrix P ([Horn and Johnson 1985](#); Corollary 7.6.5) such that*

$$P^T \widetilde{C} P = I_d \text{ and } P^T \widehat{C} P = \Lambda, \tag{12}$$

where Λ is a diagonal matrix **with diagonal elements** $\lambda_1, \lambda_2, \dots, \lambda_d$. To perform model selection, we used the correcting term in (9), where we replace $E \sum_{k=1}^d 1/\lambda_k$ with its empirical value,

$$\begin{aligned} \sum_{k=1}^d 1/\lambda_k &= \text{Tr} \left(P^{-1} \widehat{C}^{-1} (P^T)^{-1} P^T \widetilde{C} P \right) \\ &= \text{Tr}(\widehat{C}^{-1}\widetilde{C}). \end{aligned} \tag{13}$$

However, Corollary 7.6.5 in [Horn and Johnson \(1985\)](#) does not guarantee the existence of a matrix P satisfying (12). We quote the statement of the corollary.

Quote 2 (Corollary 7.6.5 in [Horn and Johnson \(1985\)](#)) *If $A \in M_n$ is positive definite and $B \in M_n$ is Hermitian, then there exists a nonsingular matrix $C \in M_n$ such that C^*BC is diagonal and $C^*AC = I$.*

Here, M_n denotes the set of all square matrices of dimension n , whose elements are complex numbers. Furthermore, the symbol $*$ denotes the Hermitian adjoint. As seen in the quote, the above corollary only guarantees that $P^T \tilde{C}P = I_d$ and $P^T \hat{C}P$ is diagonal. However, Quote 1 claims that $P^T \hat{C}P$ must be not only a diagonal matrix but also a diagonal matrix whose elements are equal to the eigenvalues of \hat{C} (See the bold part of Quote 1). This claim does not hold correct in general. Indeed, (13) is queer. Since (13) implies that $\text{Tr}(\hat{C}^{-1}) = \text{Tr}(\hat{C}^{-1}\tilde{C})$ for any unlabeled data, unlabeled data play exactly no role.

4 Modification of direct eigenvalue estimator

In this section, we consider what estimators are valid based on the idea of Chapelle et al. and which estimator is ‘good’ among valid estimators. To do so, let us calculate the bias correction factor $T^*(n, d)$ without the orthonormal assumption (7). As described before, the invariance of DEE under coordinate transformation was obtained based on the inappropriate way.

Theorem 2 *Let $\phi_1(x) \equiv 1$. Suppose that only the assumption A2 is satisfied in Theorem 1. Then $T^*(n, d)$ is exactly calculated as*

$$T^*(n, d) = \frac{1 + (1/n)E_D[\text{Tr}(\hat{C}\hat{C}^{-1})]}{1 - (d/n)}, \tag{14}$$

where $C = [C_{kk'}]$ is a $(d \times d)$ matrix with $C_{kk'} := E_x[\phi_k(x)\phi_{k'}(x)]$.

See Sect. 5.1 for its proof. The form of (14) is invariant under coordinate transformation. It is natural because the definition of $T^*(n, d)$ is invariant under coordinate transformation due to the property of LSE. There remain two unknown quantities C and $V := E_D[\hat{C}^{-1}]$ in (14). Remarkably, both of them can be estimated using only the information about covariates x . Let us define $D_0 := \{x_1, x_2, \dots, x_n\}$ and $D_x := D_0 \cup D_U$. Taking Theorem 2 into account, it is natural to consider the following class of risk estimators.

Definition 1 *(a class of valid risk estimators)* We say that a risk estimator $\hat{R}_D(d)$ is valid (in the sense of DEE) if there exists a consistent estimator¹ $\hat{H}(D_x)$ of CV such that

$$\hat{R}_D(d) = \hat{T}(n, d)L_D(f_d(\cdot; \hat{\alpha})), \quad \hat{T}(n, d) := \frac{1 + (1/n)\text{Tr}(\hat{H}(D_x))}{1 - (d/n)}.$$

We can easily understand that the resultant form of DEE is valid under some regularity conditions because \tilde{C} and \hat{C}^{-1} in (11) are statistically independent and are consistent estimators of C and V respectively. We imagine that Chapelle et al. knew the result of Theorem 2 because they implied this result in Remark 3 of Section 2.2 of [Chapelle et al. \(2002\)](#). Based on this fact, they seemingly recognized that the resultant form of DEE is valid. However, it is unclear that DEE is close to the optimal estimator in this class. In general, V is more difficult to estimate than C because V is based on the inverse matrix of \hat{C} . More concretely, \hat{C}^{-1} tends to fluctuate more largely than \hat{C} especially when n is not large enough. Hence, spending more

¹ That is, $\hat{H}(D_x)$ converges to the true value CV in probability as n and n' go to the infinity.

samples to estimate V seems to be a reasonable strategy. However, DEE spends the most of D_x (i.e., n' samples) to estimate C and spends only n samples to estimate V . Note that this strategy of DEE for estimation of CV has no necessity since the corresponding part was derived inappropriately. Therefore, let us discuss what estimators are good in among valid risk estimators. We start from the following theorem.

Theorem 3 *Let \widehat{R}_D be a valid risk estimator with $\widehat{H}(D_x)$. Define $\widehat{R}_D^*(\hat{\alpha}) := T^*(n, d) L_D(f_d \cdot; \hat{\alpha})$ with $T^*(n, d)$ in (14). If $\widehat{H}(D_x)$ depends on only unlabeled data i.e., $\widehat{H}(D_x) = \widehat{H}(D_U)$, then*

$$\begin{aligned}
 E_D \left[(R^*(d) - \widehat{R}_D(d))^2 \right] &= E_D \left[(R^*(d) - \widehat{R}_D^*(d))^2 \right] \\
 &\quad + 2 \frac{\text{bias}(\widehat{H})}{n-d} \text{cov}(\widehat{R}_D^*(d), L_D(f_d(\cdot; \hat{\alpha}(D)))) \\
 &\quad + \frac{\text{MSE}(\widehat{H})}{(n-d)^2} E_D \left[L_D(f_d(\cdot; \hat{\alpha}(D)))^2 \right]. \tag{15}
 \end{aligned}$$

Here, $\text{cov}(X, Y)$ denotes the usual covariance between X and Y and

$$\text{bias}(\text{Tr}(\widehat{H})) := E[\text{Tr}(\widehat{H}) - \text{Tr}(CV)], \quad \text{MSE}(\text{Tr}(\widehat{H})) := E \left[(\text{Tr}(\widehat{H}) - \text{Tr}(CV))^2 \right].$$

The first term of the right side of (15) is independent of the choice of \widehat{H} . It expresses error of the ideally unbiased (but unknown) risk estimator $\widehat{R}_D^*(d)$. The second term is of order $O(1/n)$ while the third term is of order $O(1/n^2)$. Therefore, it is natural to use an unbiased estimator of CV as \widehat{H} . If \widehat{H} is unbiased,

$$\begin{aligned}
 E_D \left[(R^*(d) - \widehat{R}_D(d))^2 \right] &= E_D \left[(R^*(d) - \widehat{R}_D^*(d))^2 \right] \\
 &\quad + \frac{\text{Var}(\widehat{H})}{(n-d)^2} E_D \left[L_D(f_d(\cdot; \hat{\alpha}(D)))^2 \right], \tag{16}
 \end{aligned}$$

where $\text{Var}(\widehat{H})$ denotes a variance of $\text{Tr}(\widehat{H})$. That is, as long as \widehat{H} is unbiased, \widehat{H} having the smallest $\text{Var}(\widehat{H})$ gives the best performance. This fact motivates us to consider the following estimator. Let us divide the unlabeled data set D_U into two data sets $D_U^1 := \{x'_1, x'_2, \dots, x'_{n_1}\}$ and $D_U^2 := \{x'_{n_1+1}, x'_{n_1+2}, \dots, x'_{n_1+n_2}\}$ for estimating C and V respectively. Furthermore, we divide D_U^2 into $B_2 := \lfloor n_2/n \rfloor$ subsets such that the b -th subset is

$$D_b := \left\{ x'_{(b-1) \cdot n + 1 + n_1}, x'_{(b-1) \cdot n + 2 + n_1}, \dots, x'_{b \cdot n + n_1} \right\}.$$

As a result, each D_b is an i.i.d. copy of D_0 . Define \widehat{C}_b as an empirical correlation matrix of $\phi(x) = (\phi_1(x), \phi_2(x), \dots, \phi_d(x))^T$ based on D_b . Then, it is natural to estimate V as

$$\widehat{V} := \frac{1}{B_2} \sum_{b=1}^{B_2} \widehat{C}_b^{-1}.$$

On the other hand, we can estimate C using D_U^1 simply as

$$\widehat{C}_+ := \frac{1}{n_1} \left(\sum_{j=1}^{n_1} \phi(x'_j) \phi(x'_j)^T \right).$$

Table 1 Variation of mDEE. This table expresses which data are used to estimate C and V

	Data used for \widehat{C}_+	Data used for \widehat{V}
mDEE1	D_U^1	D_U^2
mDEE2	D_U^1	D_U
mDEE3	D_U	D_U

Then, we simply make $\widehat{H}_1 := \widehat{C}_+ \widehat{V}$. The resultant risk estimator is

$$\widehat{R}_D^1 := \frac{1 + (1/n)\text{Tr}(\widehat{H}_1)}{1 - (d/n)} L_D(f_d(\cdot; \hat{\alpha}(D))). \tag{17}$$

We refer to this modified version of DEE as mDEE1. There are other possible variations depending on how to estimate C and V based on unlabeled data. We prepare the three candidates shown in Table 1. Both mDEE2 and mDEE3 construct \widehat{C}_+ , \widehat{V} and \widehat{H} in the same way as mDEE1. We write \widehat{H} used for mDEE1-3 as \widehat{H}_1 , \widehat{H}_2 and \widehat{H}_3 . While mDEE1 has no overlapped samples between \widehat{C}_+ and \widehat{V} , mDEE3 uses all unlabeled data to estimate both C and V . The other estimator mDEE2 is their intermediate. By checking some properties of these estimators, we have the following theorem.

Theorem 4 Assume that both n_1 and n_2 can be divided by n . Let $B_1 := n_1/n$, $B_2 := n_2/n$ and $B := n'/n$. Let μ and ν be column vectors obtained by vectorizing C and V respectively. Similarly, we vectorize \widehat{C}_a and \widehat{C}_b^{-1} as $\widehat{\mu}_a$ and $\widehat{\nu}_b$. We also define $\widehat{\mu}$ and $\widehat{\nu}$ as i.i.d. copies of $\widehat{\mu}_a$ and $\widehat{\nu}_b$. Then,

$$\begin{aligned} \text{bias}(\widehat{H}_1) &= 0, \text{ bias}(\widehat{H}_2) = \text{bias}(\widehat{H}_3) = \frac{d - \text{Tr}(CV)}{B}, \\ \text{Var}(\text{Tr}(\widehat{H}_1)) &= \frac{\text{Tr}(\text{Var}(\widehat{\mu})\text{Var}(\widehat{\nu}))}{B_1 B_2} + \frac{\text{Tr}(\text{Var}(\widehat{\nu})\mu\mu^T)}{B_2} + \frac{\text{Tr}(\text{Var}(\widehat{\mu})\nu\nu^T)}{B_1}. \end{aligned}$$

Furthermore, if we fix B (or equivalently n and n'), the variance of $\text{Tr}(\widehat{H}_1)$ is minimized by the ceiling or flooring of

$$B_1^* = \begin{cases} \left(\frac{a_1 - \sqrt{a_1 a_2}}{a_1 - a_2} \right) B & \text{if } a_1 \neq a_2 \\ B/2 & \text{otherwise} \end{cases}, \tag{18}$$

where

$$a_1 := \frac{\text{Tr}(\text{Var}(\widehat{\mu})\text{Var}(\widehat{\nu}))}{B} + \text{Tr}(\text{Var}(\widehat{\mu})\nu\nu^T), \quad a_2 := \frac{\text{Tr}(\text{Var}(\widehat{\mu})\text{Var}(\widehat{\nu}))}{B} + \text{Tr}(\text{Var}(\widehat{\nu})\mu\mu^T).$$

See Sect. 5.3 for its proof. The estimator mDEE1 seems to be the most reasonable estimator because its first order term $O(1/n)$ vanishes. Furthermore, $\text{MSE}(\widehat{H}_1) = \text{Var}(\text{Tr}(\widehat{H}_1))$ can be calculated explicitly as in Theorem 4. This is beneficial because the optimal balance of sample numbers used to estimate C and V , i.e., B_1^* , can be estimated as follows. By the above theorem, it suffices to estimate the quantities a_1 and a_2 in order to estimate B_1^* . Both quantities can be calculated if we know μ , ν , $\text{Var}(\widehat{\mu})$ and $\text{Var}(\widehat{\nu})$. We estimate them such as

$$\begin{aligned} \bar{\mu} &= \frac{1}{B} \sum_{b=1}^B \hat{\mu}_b, \quad \bar{v} = \frac{1}{B} \sum_{b=1}^B \hat{v}_b, \\ \overline{\text{Var}}(\hat{\mu}) &= \frac{1}{B-1} \sum_{b=1}^B \left(\hat{\mu}_b \hat{\mu}_b^T - \bar{\mu} \bar{\mu}^T \right), \quad \overline{\text{Var}}(\hat{v}) = \frac{1}{B-1} \sum_{b=1}^B \left(\hat{v}_b \hat{v}_b^T - \bar{v} \bar{v}^T \right). \end{aligned}$$

Thus, we propose to choose the optimal B_1 as the rounded value of (18) with a_1 and a_2 calculated by using the above empirical estimates.

In contrast to the case of mDEE1, the estimators mDEE2 and mDEE3 admit the bias. Therefore, we should discuss their performance through (15) instead (16). Then, we must care about MSE of \hat{H} . Recall that MSE can be decomposed into bias and variance terms [(for example, see Hastie et al. (2001)], i.e.,

$$\begin{aligned} \text{MSE}(\hat{H}) &= E \left[(\text{Tr}(\hat{H}) - \text{Tr}(CV))^2 \right] \\ &= E \left[(\text{Tr}(\hat{H}) - E[\text{Tr}(\hat{H})])^2 \right] + (E[\text{Tr}(\hat{H})] - \text{Tr}(CV))^2 \\ &= \text{Var}(\text{Tr}(\hat{H})) + \text{bias}(\text{Tr}(\hat{H}))^2. \end{aligned}$$

The estimators mDEE2 and mDEE3 are developed to decrease the variance of \hat{H} at cost of the bias increase. This is effective when the variance is much larger than bias. If the bias increases, the second term of (15) gets larger. When we can obtain unlabeled data as many as we like, $\text{bias}(\text{Tr}(\hat{H}))$ can be decreased to zero as $B \rightarrow \infty$ by Theorem 4. MSE also decreases to zero as $B \rightarrow \infty$ because of the consistency of \hat{H} . Nevertheless, if the number of unlabeled data is not enough, we have to take care which is better mDEE1 or mDEE2-3.

Many readers may think that the variance of $\text{Tr}(\hat{H}_2)$ should be calculated to estimate the optimal B_1 for mDEE2. Surely, it is possible. However, the resultant form is excessively complicated and includes the third and the fourth cross moments. Hence, the resultant way to choose B_1 is also computationally expensive and instable when d gets large. Thus, we do not employ the exact variance evaluation and survey the performance of mDEE2 by numerical simulations.

Finally, we review again DEE. DEE does not satisfy the assumption of Theorem 3 because \hat{H} of DEE utilizes D_0 . When \hat{H} is allowed to depend on D_0 , then we cannot obtain any clear result like Theorem 3. Hence, we cannot compare DEE and mDEE through Theorem 3. However, DEE looks similar to mDEE1 when $B_1 = B - 1$ is selected. Since B_1 of mDEE1 is optimized by the above way, mDEE1 does not necessarily behave similarly to DEE. Actually, it will be turned out by numerical experiments that the estimated B_1^* for mDEE1 tends to be very small compared to B . This fact indicates that the most unlabeled data should be used to estimate V . As a result, DEE does not exploit available data efficiently.

5 Proofs of Theorems

In this section, we provide proofs to all original theorems.

5.1 Proof of Theorem 2

Proof We do not need to trace the whole derivation of DEE. The result for non-orthonormal cases is obtained by using (9) as follows. For convenience, let $\phi(x) := (\phi_1(x), \phi_2(x), \dots, \phi_d(x))^T$ for each d . Because the basis is not orthonormal, $C = E_x[\phi(x)\phi(x)^T]$ is not an identity matrix. Using C , define

$$\phi'(x) := C^{-1/2}\phi(x).$$

Then, $\{\phi'_k(x) | k = 1, 2, \dots, d\}$ comprises an orthonormal basis of $\text{Span}(\phi)$. Note that the LSE estimate of regression function does not change if we replace the original basis $\{\phi_k(x)\}$ with this orthonormal basis $\{\phi'_k(x)\}$. Therefore, using the basis $\{\phi'_k(x)\}$, we obtain the same result as (14) except the replacement of \widehat{C} with $\widehat{C}' = (1/n)(\Phi')^T \Phi'$, where Φ' is a matrix whose (i, k) element is $\phi'_k(x_i)$. Noting that $\Phi' = \Phi C^{-1/2}$, we can rewrite \widehat{C}' as

$$\widehat{C}' = \frac{1}{n} C^{-1/2} \Phi^T \Phi C^{-1/2} = C^{-1/2} \widehat{C} C^{-1/2}.$$

Substituting this into (14), we obtain a new version of (14) as

$$T^*(n, d) = \frac{1 + (1/n)\text{Tr}(E_D [C^{1/2} \widehat{C}^{-1} C^{1/2}])}{1 - (d/n)} = \frac{1 + (1/n)\text{Tr}(C E_D [\widehat{C}^{-1}])}{1 - (d/n)}$$

for non-orthonormal cases. □

5.2 Proof of Theorem 3

Proof The left side of (15) is calculated as

$$E_D \left[(R^*(d) - \widehat{R}_D(d))^2 \right] = E_D \left[(R^*(d) - \widehat{R}_D^*(d))^2 + (\widehat{R}_D^*(d) - \widehat{R}_D(d))^2 + 2(R^*(d) - \widehat{R}_D^*(d))(\widehat{R}_D^*(d) - \widehat{R}_D(d)) \right]. \tag{19}$$

The last term is calculated as

$$\begin{aligned} & E \left[(R^*(d) - \widehat{R}_D^*(d)) (\widehat{R}_D^*(d) - \widehat{R}_D(d)) \right] \\ &= E \left[(R^*(d) - \widehat{R}_D^*(d)) (T^*(n, d) - \widehat{T}(n, d)) L_D(f_d(\cdot; \hat{\alpha}(D))) \right] \\ &= E \left[(R^*(d) - \widehat{R}_D^*(d)) L_D(f_d(\cdot; \hat{\alpha}(D))) \right] E \left[(T^*(n, d) - \widehat{T}(n, d)) \right] \\ &= \text{cov}(\widehat{R}_D^*(d), L_D(f_d(\cdot; \hat{\alpha}(D)))) E \left[(\widehat{T}(n, d) - T^*(n, d)) \right]. \end{aligned}$$

The second last equality is obtained since $\widehat{T}(n, d)$ is statistically independent of D ($\widehat{T}(n, d)$ depends only on D_U). The second term of (19) is calculated as

$$\begin{aligned} E \left[(\widehat{R}_D^*(d) - \widehat{R}_D(d))^2 \right] &= E \left[(T^*(n, d) - \widehat{T}(n, d))^2 L_D(f_d(\cdot; \hat{\alpha}(D)))^2 \right] \\ &= E \left[(T^*(n, d) - \widehat{T}(n, d))^2 \right] E \left[L_D(f_d(\cdot; \hat{\alpha}(D)))^2 \right]. \end{aligned}$$

The proof is completed by noting that

$$\widehat{T}(n, d) - T^*(n, d) = \frac{1 + \frac{1}{n} \text{Tr}(\widehat{H}) - (1 + \frac{1}{n} \text{Tr}(CV))}{1 - (d/n)} = \frac{\text{Tr}(\widehat{H}) - \text{Tr}(CV)}{n - d}.$$

□

5.3 Proof of Theorem 4

Proof Let us partition the whole unlabeled data set D_U into subsets consisting of n samples. We write them as D_1, D_2, \dots, D_B . Then, we can write $D_U^1 = \cup_{a=1}^{B_1} D_a$ and $D_U^2 = \cup_{b=B_1+1}^B D_b$. As before, each empirical correlation matrix based on D_b is denoted by

\widehat{C}_b . The bias of \widehat{H}_1 trivially vanishes because of the statistical independence between \widehat{C}_+ and \widehat{V} . As for mDEE2, it holds that

$$\widehat{H}_2 = \left(\frac{1}{B_1} \sum_{a=1}^{B_1} \widehat{C}_a \right) \left(\frac{1}{B} \sum_{b=1}^B \widehat{C}_b^{-1} \right) = \frac{1}{B_1 B} \sum_{a=1}^{B_1} \sum_{b=1}^B \widehat{C}_a \widehat{C}_b^{-1}.$$

Taking expectation, we have

$$\begin{aligned} E[\widehat{H}_2] &= \frac{1}{B_1 B} \sum_{a=1}^{B_1} \sum_{b=1}^B E[\widehat{C}_a \widehat{C}_b^{-1}] = \frac{1}{B_1 B} \sum_{a=1}^{B_1} \sum_{b=1}^B (\delta_{ab} I_d + (1 - \delta_{ab}) CV) \\ &= \frac{1}{B_1 B} (B_1 I_d + (B B_1 - B_1) CV) = \frac{1}{B} (I_d + (B - 1) CV). \end{aligned}$$

Hence, the bias of $\text{Tr}(\widehat{H}_2)$ is

$$E[\text{Tr}(\widehat{H}_2) - \text{Tr}(CV)] = \frac{d - \text{Tr}(CV)}{B}.$$

This does not depend on B_1 , so that $\text{Tr}(\widehat{H}_3)$ has the same bias. Next, we calculate the variance of $\text{Tr}(\widehat{H}_1)$. Let $\mathcal{B}_1 = \{1, 2, \dots, B_1\}$ and $\mathcal{B}_2 = \{B_1 + 1, B_1 + 2, \dots, B\}$. Since \mathcal{B}_1 and \mathcal{B}_2 are disjoint, $E\text{Tr}(\widehat{C}_a \widehat{C}_b^{-1}) = \mu^T v$ for any $a \in \mathcal{B}_1$ and $b \in \mathcal{B}_2$. Hence, we have

$$\begin{aligned} \text{Var}(\text{Tr}(\widehat{H}_1)) &= E\left(\frac{1}{B_1 B_2} \sum_{a \in \mathcal{B}_1} \sum_{b \in \mathcal{B}_2} \text{Tr}(\widehat{C}_a \widehat{C}_b^{-1}) - \mu^T v\right)^2 \\ &= E\left(\frac{1}{B_1 B_2} \sum_{a \in \mathcal{B}_1} \sum_{b \in \mathcal{B}_2} \hat{\mu}_a^T \hat{v}_b - \mu^T v\right)^2 \\ &= \frac{1}{B_1^2 B_2^2} E\left(\sum_{a \in \mathcal{B}_1} \sum_{b \in \mathcal{B}_2} (\hat{\mu}_a^T \hat{v}_b - \mu^T v)\right)^2 \\ &= \frac{1}{B_1^2 B_2^2} \sum_{a \in \mathcal{B}_1} \sum_{b \in \mathcal{B}_2} \sum_{c \in \mathcal{B}_1} \sum_{d \in \mathcal{B}_2} E(\hat{\mu}_a^T \hat{v}_b - \mu^T v)(\hat{\mu}_c^T \hat{v}_d - \mu^T v). \end{aligned}$$

We will make a case argument for the terms in the last summation. If $c \neq a$ and $b \neq d$, both factors are independent of each other. Hence, we have

$$E(\hat{\mu}_a^T \hat{v}_b - \mu^T v)(\hat{\mu}_c^T \hat{v}_d - \mu^T v) = 0.$$

If $c = a$ and $d \neq b$, we have

$$\begin{aligned} E(\hat{\mu}_a^T \hat{v}_b - \mu^T v)(\hat{\mu}_c^T \hat{v}_d - \mu^T v) &= E(\hat{\mu}_a^T \hat{v}_b - \mu^T v)(\hat{\mu}_a^T \hat{v}_d - \mu^T v) \\ &= E(\hat{\mu}_a^T v - \mu^T v)(\hat{\mu}_a^T v - \mu^T v) \\ &= E(\hat{\mu}_a^T - \mu^T)v(\hat{\mu}_a^T - \mu^T)v \\ &= \text{Tr}(\text{Var}(\hat{\mu})v v^T) \end{aligned}$$

Similarly, if $c \neq a$ and $d = b$, we have

$$E(\hat{\mu}_a^T \hat{v}_b - \mu^T v)(\hat{\mu}_c^T \hat{v}_d - \mu^T v) = \text{Tr}(\mu \mu^T \text{Var}(\hat{v})).$$

Finally, if $c = a$ and $b = d$,

$$\begin{aligned} E\left(\hat{\mu}_a^T \hat{v}_b - \mu^T v\right)\left(\hat{\mu}_c^T \hat{v}_d - \mu^T v\right) &= E\left(\hat{\mu}_a^T \hat{v}_b - \mu^T v\right)^2 = E\left(\hat{\mu}_a^T (\hat{v}_b - v) + (\hat{\mu}_a^T - \mu^T)v\right)^2 \\ &= E\left(\left(\hat{\mu}_a^T - \mu^T\right)(\hat{v}_b - v) + \mu^T(\hat{v}_b - v) + (\hat{\mu}_a^T - \mu^T)v\right)^2. \end{aligned}$$

Since the three terms in the last side are not correlated to each other, we have

$$\begin{aligned} E\left(\hat{\mu}_a^T \hat{v}_b - \mu^T v\right)^2 &= E\left(\left(\hat{\mu}_a^T - \mu^T\right)(\hat{v}_b - v)\right)^2 + E\left(\mu^T(\hat{v}_b - v)\right)^2 + E\left(\left(\hat{\mu}_a^T - \mu^T\right)v\right)^2 \\ &= \text{Tr}(\text{Var}(\hat{\mu})\text{Var}(\hat{v})) + \text{Tr}(\mu\mu^T\text{Var}(\hat{v})) + \text{Tr}(\text{Var}(\hat{\mu})vv^T). \end{aligned}$$

Therefore, we have

$$\begin{aligned} \text{Var}(\text{Tr}(\hat{H}_1)) &= \frac{1}{B_1^2 B_2^2} \left(B_1 B_2 \text{Tr}(\text{Var}(\hat{\mu})\text{Var}(\hat{v})) + B_1^2 B_2 \text{Tr}(\mu\mu^T\text{Var}(\hat{v})) + B_1 B_2^2 \text{Tr}(\text{Var}(\hat{\mu})vv^T) \right) \\ &= \frac{1}{B_1 B_2} \left(\text{Tr}(\text{Var}(\hat{\mu})\text{Var}(\hat{v})) + B_1 \text{Tr}(\mu\mu^T\text{Var}(\hat{v})) + B_2 \text{Tr}(\text{Var}(\hat{\mu})vv^T) \right). \end{aligned}$$

Finally, we minimize the variance in terms of B_1 . Since B is fixed, $B_2 = B - B_1$. Using $1/(B(B - B_1)) = (1/B)(1/B + 1/(B - B_1))$, $\text{Var}(\text{Tr}(\hat{H}_1))$ is rewritten as

$$\begin{aligned} \text{Var}(\text{Tr}(\hat{H}_1)) &= \frac{1}{B_1} \left(\frac{\text{Tr}(\text{Var}(\hat{\mu})\text{Var}(\hat{v}))}{B} + \text{Tr}(\text{Var}(\hat{\mu})vv^T) \right) \\ &\quad + \frac{1}{B - B_1} \left(\frac{\text{Tr}(\text{Var}(\hat{\mu})\text{Var}(\hat{v}))}{B} + \text{Tr}(\text{Var}(\hat{v})\mu\mu^T) \right) \\ &= \frac{a_1}{B_1} + \frac{a_2}{B - B_1}. \end{aligned}$$

By regarding $\text{Var}(\text{Tr}(\hat{H}_1))$ as a continuous function of B_1 and differentiating it,

$$\frac{d}{dB_1} \text{Var}(\text{Tr}(\hat{H}_1)) = \frac{a_2}{(B - B_1)^2} - \frac{a_1}{B_1^2}.$$

By setting this to zero, we obtain the second order equation of B_1 . Its solution is

$$\left(\frac{a_1 \pm \sqrt{a_1 a_2}}{a_1 - a_2} \right) B.$$

It is easy to check that $(a_1 + \sqrt{a_1 a_2})/(a_1 - a_2) \notin (0, 1)$ while $(a_1 - \sqrt{a_1 a_2})/(a_1 - a_2) \in (0, 1)$. Since $\text{Var}(\text{Tr}(\hat{H}_1))$ is convex in $B_1 \in (0, B)$, the minimum is attained by $(a_1 - \sqrt{a_1 a_2})/(a_1 - a_2)$. Therefore, the optimal integer B_1 is its ceiling or floor. \square

6 Numerical experiments

By numerical experiments, we compare the performance of mDEE with the original DEE and ADJ and other existing methods. We basically employ the same setting as [Chapelle et al. \(2002\)](#). Define Fourier basis functions $\phi_k : \mathfrak{R} \rightarrow \mathfrak{R}$ as

$$\phi_1(x) = 1, \phi_{2p}(x) = \sqrt{2} \cos(px), \phi_{2p+1}(x) = \sqrt{2} \sin(px).$$

Table 2 This table summarizes which table shows the result of which experiment

Table	3	4	5	6	7	8
Regression function	sinc	sinc	sinc	step	step	step
n	10	20	50	10	20	50

The regression model $f_d : \mathfrak{R}^M \rightarrow \mathfrak{R}$ is defined by

$$f_d(x; \alpha) = \sum_{m=1}^M \sum_{k=1}^d \alpha_k \phi_k(x_m), \tag{20}$$

where x_m denotes the m -th component of x . Note that $f_d(x; \alpha)$ cannot span $L^2(\mathcal{X})$ even with $d \rightarrow \infty$ when $M > 1$. For each $d = 1, 2, \dots, \bar{d}$, we compute LSE² $\hat{\alpha}(D)$ for model \mathcal{M}_d . Then, we calculate various risk estimators (model selection criteria) for each d and choose \hat{d} minimizing it. The performance of each risk estimator is measured by so-called *regret* defined by the log ratio of risk to the best model:

$$\log \left(\frac{\widehat{R}_D(f_{\hat{d}}(x; \hat{\alpha}(D)))}{\min_d \widehat{R}_D(f_d(x; \hat{\alpha}(D)))} \right). \tag{21}$$

Here, $\widehat{R}_D(f_d(\cdot; \hat{\alpha}(d)))$ expresses a test error, $\widehat{R}_D(f_d(x; \hat{\alpha}(d))) := \frac{1}{\bar{n}} \sum_{i=1}^{\bar{n}} (y_i'' - f_d(x_i''; \hat{\alpha}(d)))^2$, where the test data $\{(x_i'', y_i'') \mid i = 1, 2, \dots, \bar{n}\}$ are generated from the same distribution as the training data. We compare mDEE1-3 with FPE (Akaike 1970), cAIC (Sugiura 1978) and cv (five-fold cross-validation) in addition to DEE and ADJ. In calculation of mDEE1, B_1 (or n_1) was chosen according to the way described in Sect. 4. We also used the same B_1 for mDEE2.

6.1 Synthetic data

First, we conduct the same experiments as that of Chapelle et al. (2002) as follows. We prepare the following two true regression functions,

$$\text{sinc function } f_1(x) = \sin(4x)/4x, \quad \text{step function } f_2(x) = I(x > 0),$$

where $I(\cdot)$ is an indicator function returning 1 if its argument is true and zero otherwise. The sinc function can be approximated well by fewer terms in (20) compared to the step function. The training data are generated according to the regression model in (1) with the above regression functions. The noise ξ_i is subject to $N(\xi_i; 0, \sigma^2)$ which denotes the normal distribution with mean 0 and variance σ^2 . We prepare $n = 10, 20, 50$ training samples and $n' = 1500$ unlabeled data. Covariates x_i are generated from $N(0, \bar{\sigma}^2)$ independently in contrast to Chapelle et al. (2002). Note that the above basis functions are not orthonormal with respect to $p(x)$ in this case. The model candidate number \bar{d} was chosen as $\bar{d} = 8$ for $n = 10, \bar{d} = 15$ for $n = 20$ and $\bar{d} = 23$ for $n = 50$. The number of test data is set as $\bar{n} = 1000$ in all simulations. We conducted a series of experiments by varying the regression function and the sample number n summarized in Table 2. In each experiment, σ^2 is varied among $\{0.01, 0.05, 0.1, 0.2, 0.3, 0.4\}$. The experiments were repeated 1000 times. The results are

² To avoid the singularity of $\Phi^T \Phi$, we used Ridge estimator. However, its regularization coefficient is set to $\lambda = 10^{-9}$. Therefore, it almost works like LSE.

Table 3 Median (IQR) of regret of each model selection method when the true regression function is $f_1(x)$, $n = 10$

σ^2	0.01	0.05	0.1	0.2	0.3	0.4
FPE	1.030 (2.720)	0.888 (3.070)	0.880 (2.780)	0.707 (2.690)	0.697 (2.540)	0.650 (2.910)
cAIC	1.250 (1.050)	0.452 (0.456)	0.281 (0.271)	0.114 (0.160)	0.084 (0.127)	0.058 (0.116)
ADJ	0.336 (0.949)	0.190 (0.492)	0.197 (0.379)	0.116 (0.277)	0.107 (0.296)	0.103 (0.287)
cv	0.929 (1.160)	0.427 (0.548)	0.280 (0.373)	0.146 (0.253)	0.102 (0.214)	0.085 (0.252)
DEE	0.497 (1.390)	0.361 (0.718)	0.298 (0.503)	0.180 (0.358)	0.150 (0.393)	0.113 (0.375)
mDEE1	1.190 (1.050)	0.483 (0.510)	0.300 (0.340)	0.144 (0.215)	0.102 (0.171)	0.077 (0.170)
mDEE2	1.190 (1.050)	0.483 (0.511)	0.300 (0.341)	0.144 (0.215)	0.102 (0.170)	0.077 (0.170)
mDEE3	1.210 (1.050)	0.479 (0.510)	0.299 (0.330)	0.140 (0.212)	0.103 (0.169)	0.076 (0.162)

Table 4 Median (IQR) of regret of each model selection method when the true regression function is $f_1(x)$, $n = 20$

σ^2	0.01	0.05	0.1	0.2	0.3	0.4
FPE	0.901 (3.630)	0.626 (2.910)	0.562 (2.760)	0.469 (3.180)	0.340 (2.320)	0.325 (2.380)
cAIC	0.342 (0.620)	0.204 (0.537)	0.265 (0.393)	0.236 (0.214)	0.139 (0.146)	0.112 (0.127)
ADJ	0.254 (0.660)	0.164 (0.478)	0.155 (0.324)	0.151 (0.217)	0.104 (0.178)	0.099 (0.158)
cv	0.335 (0.698)	0.220 (0.518)	0.215 (0.390)	0.199 (0.236)	0.134 (0.185)	0.121 (0.167)
DEE	0.179 (0.619)	0.162 (0.433)	0.148 (0.341)	0.181 (0.249)	0.152 (0.199)	0.132 (0.175)
mDEE1	0.462 (0.468)	0.179 (0.493)	0.211 (0.375)	0.205 (0.220)	0.141 (0.160)	0.124 (0.151)
mDEE2	0.462 (0.467)	0.178 (0.494)	0.213 (0.375)	0.205 (0.220)	0.140 (0.159)	0.124 (0.149)
mDEE3	0.469 (0.427)	0.181 (0.500)	0.215 (0.379)	0.210 (0.218)	0.139 (0.152)	0.123 (0.150)

Table 5 Median (IQR) of regret of each model selection method when the true regression function is $f_1(x)$, $n = 50$

σ^2	0.01	0.05	0.1	0.2	0.3	0.4
FPE	0.036 (0.247)	0.068 (0.197)	0.064 (0.207)	0.055 (0.188)	0.081 (0.210)	0.077 (0.161)
cAIC	0.002 (0.033)	0.041 (0.111)	0.040 (0.071)	0.037 (0.096)	0.055 (0.133)	0.068 (0.109)
ADJ	0.022 (0.120)	0.060 (0.130)	0.052 (0.124)	0.058 (0.170)	0.092 (0.160)	0.080 (0.129)
cv	0.011 (0.075)	0.051 (0.118)	0.048 (0.095)	0.043 (0.123)	0.073 (0.162)	0.071 (0.118)
DEE	0.009 (0.063)	0.042 (0.112)	0.047 (0.090)	0.038 (0.102)	0.053 (0.132)	0.064 (0.114)
mDEE1	0.005 (0.041)	0.028 (0.102)	0.040 (0.076)	0.035 (0.086)	0.048 (0.120)	0.061 (0.106)
mDEE2	0.005 (0.041)	0.028 (0.101)	0.040 (0.076)	0.035 (0.088)	0.048 (0.121)	0.061 (0.106)
mDEE3	0.005 (0.042)	0.027 (0.099)	0.040 (0.076)	0.036 (0.088)	0.048 (0.120)	0.062 (0.107)

Table 6 Median (IQR) of regret of each model selection method when the true regression function is $f_2(x)$, $n = 10$

σ^2	0.01	0.05	0.1	0.2	0.3	0.4
FPE	1.180 (3.650)	0.936 (3.470)	0.887 (3.390)	0.737 (3.120)	0.567 (2.580)	0.581 (2.910)
cAIC	0.074 (0.563)	0.145 (0.618)	0.309 (0.551)	0.255 (0.326)	0.199 (0.259)	0.150 (0.232)
ADJ	0.121 (0.471)	0.142 (0.545)	0.150 (0.503)	0.159 (0.406)	0.148 (0.326)	0.145 (0.320)
cv	0.075 (0.447)	0.096 (0.486)	0.086 (0.469)	0.152 (0.372)	0.168 (0.318)	0.156 (0.288)
DEE	0.146 (0.628)	0.130 (0.522)	0.118 (0.508)	0.185 (0.427)	0.190 (0.358)	0.178 (0.333)
mDEE1	0.023 (0.215)	0.013 (0.194)	0.007 (0.257)	0.052 (0.286)	0.133 (0.282)	0.124 (0.253)
mDEE2	0.023 (0.215)	0.013 (0.197)	0.008 (0.259)	0.052 (0.286)	0.133 (0.282)	0.124 (0.253)
mDEE3	0.020 (0.198)	0.012 (0.188)	0.008 (0.259)	0.052 (0.288)	0.129 (0.282)	0.124 (0.250)

Table 7 Median (IQR) of regret of each model selection method when the true regression function is $f_2(x)$, $n = 20$

σ^2	0.01	0.05	0.1	0.2	0.3	0.4
FPE	2.660 (5.540)	1.390 (4.620)	0.910 (3.990)	0.587 (3.600)	0.459 (3.050)	0.402 (2.670)
cAIC	0.134 (0.186)	0.052 (0.163)	0.040 (0.150)	0.033 (0.219)	0.030 (0.263)	0.064 (0.250)
ADJ	0.130 (0.220)	0.091 (0.242)	0.075 (0.217)	0.089 (0.311)	0.111 (0.302)	0.122 (0.279)
cv	0.130 (0.184)	0.079 (0.229)	0.065 (0.217)	0.068 (0.273)	0.079 (0.287)	0.105 (0.268)
DEE	0.181 (0.317)	0.113 (0.315)	0.078 (0.247)	0.080 (0.279)	0.078 (0.290)	0.075 (0.262)
mDEE1	0.133 (0.177)	0.073 (0.191)	0.049 (0.164)	0.040 (0.193)	0.026 (0.205)	0.038 (0.225)
mDEE2	0.133 (0.177)	0.073 (0.191)	0.049 (0.164)	0.040 (0.193)	0.025 (0.205)	0.037 (0.226)
mDEE3	0.134 (0.173)	0.073 (0.190)	0.047 (0.155)	0.039 (0.191)	0.024 (0.203)	0.030 (0.223)

Table 8 Median (IQR) of regret of each model selection method when the true regression function is $f_2(x)$, $n = 50$

σ^2	0.01	0.05	0.1	0.2	0.3	0.4
FPE	0.522 (1.550)	0.273 (1.120)	0.169 (0.571)	0.087 (0.342)	0.077 (0.274)	0.072 (0.274)
cAIC	0.140 (0.217)	0.095 (0.105)	0.071 (0.077)	0.053 (0.060)	0.028 (0.075)	0.013 (0.091)
ADJ	0.093 (0.125)	0.076 (0.095)	0.058 (0.089)	0.049 (0.070)	0.034 (0.106)	0.039 (0.152)
cv	0.122 (0.153)	0.092 (0.101)	0.072 (0.088)	0.051 (0.068)	0.031 (0.093)	0.024 (0.128)
DEE	0.150 (0.246)	0.100 (0.131)	0.080 (0.109)	0.058 (0.081)	0.038 (0.106)	0.023 (0.137)
mDEE1	0.116 (0.156)	0.084 (0.105)	0.071 (0.085)	0.055 (0.069)	0.036 (0.087)	0.020 (0.118)
mDEE2	0.116 (0.155)	0.085 (0.105)	0.071 (0.085)	0.055 (0.070)	0.036 (0.087)	0.020 (0.118)
mDEE3	0.112 (0.146)	0.084 (0.104)	0.071 (0.084)	0.055 (0.070)	0.036 (0.087)	0.019 (0.116)

Table 9 Properties of real world data sets and experimental setting

Data set	Dim(x)	Total data number	n'	Source
Concrete compressive strength (concrete)	8	1030	800	UCI
NO2 (NO2)	7	500	350	StatLib
Bank 8nm (bank)	8	8192	1300	DELVE
Pumadyn family 8 nm (puma)	8	8192	1300	DELVE
Heating energy efficiency (eeheat)	8	768	550	UCI
Cooling energy efficiency (eecool)	8	768	550	UCI
Abalone	7	4177	1300	UCI

shown in Tables 3, 4, 5, 6, 7 and 8. These tables show the median and IQR (InterQuartile Range) of regret of each method.

As for these synthetic data, the performance of mDEE1-mDEE3 are almost same. Hence, we do not discriminate them here. When the true regression function is easy to estimate (i.e., f_1) and the noise variance σ^2 is small enough, DEE performs comparatively or a little bit dominated mDEE. Otherwise, all mDEE dominated DEE. Especially, mDEE is more stable than DEE because IQR of mDEE is usually smaller than that of DEE. Compared to ADJ, mDEE also performed better than ADJ except the case where σ^2 is small and the true regression function is f_1 . This observation holds to some extent in comparison with other methods. As a whole, mDEE is apt to be dominated by existing methods when the regression function is easy to estimate and the noise variance is almost equal to zero. In other cases, mDEE usually dominated other methods. Finally, we remark that the estimated B_1 for mDEE1 took its value usually around 1 – 20. This fact indicates that $V = E_D[\widehat{C}^{-1}]$ requires much more samples to estimate than C .

6.2 Real world data

We conducted the similar experiments on some real-world data sets from UCI (Bache and Lichman 2013), StatLib and DELVE benchmark databases as shown in Table 9. We used again (20) as the regression model. The number of model candidates \bar{d} was determined by $\lceil (n - 1)/M \rceil$. We varied n as $n = 20, 50$ in experiments. The total number of unlabeled data n' is described in Table 9. The test data number \bar{n} was set to ‘total data number’ – $(n + n')$ in each experiment.

The results are shown in Figs. 1 and 2. First, we should mention that mDEE seemed to work poorly for the data sets “eeheat” and “eecool.” These data sets include discrete covariates taking only a few values. Thus, there are some sub data sets D_b in which the above covariates take the exactly same value. In such cases, \widehat{C}_b^{-1} based on such D_b diverges to infinity. To see this, we show the histogram of $\text{Tr}(\widehat{C}_+ \widehat{C}_b^{-1})$ of mDEE3 for “eeheat” data with $n = 10$ in Fig. 3. From Fig. 3, we can see that some values of them take extremely large values. There are some ways to avoid this difficulty. The simplest way is to replace the empirical mean $\frac{1}{B+1} \sum_{b=0}^B \text{Tr}(\widehat{C}_+ \widehat{C}_b^{-1})$ in (17) with the median of $\left\{ \text{Tr}(\widehat{C}_+ \widehat{C}_0^{-1}), \text{Tr}(\widehat{C}_+ \widehat{C}_1^{-1}), \dots, \text{Tr}(\widehat{C}_+ \widehat{C}_B^{-1}) \right\}$. Applying this idea to mDEE3, we obtain a new criterion referred to as rmDEE (robust mDEE). Each panel of “eeheat” and “eecool” in Fig. 2 contains the result of rmDEE instead mDEE2. From Fig. 2, we can see that rmDEE

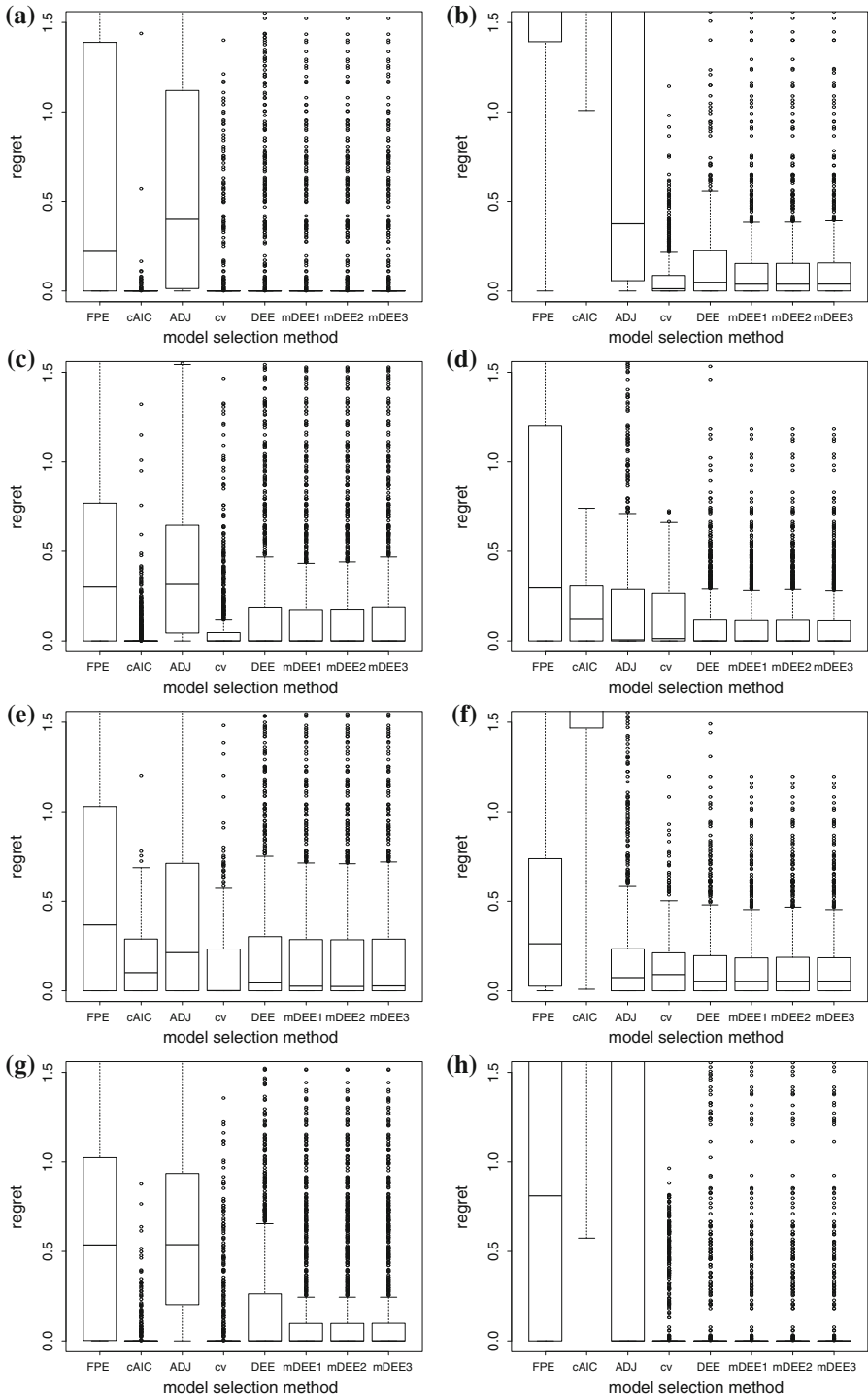


Fig. 1 Boxplot of regret for real-world data sets. **a** data: concrete, $n = 20$. **b** data: concrete, $n = 50$. **c** data: NO₂, $n = 20$. **d** data: NO₂, $n = 50$. **e** data: bank, $n = 20$. **f** data: bank, $n = 50$. **g** data: puma, $n = 20$. **h** data: puma, $n = 50$

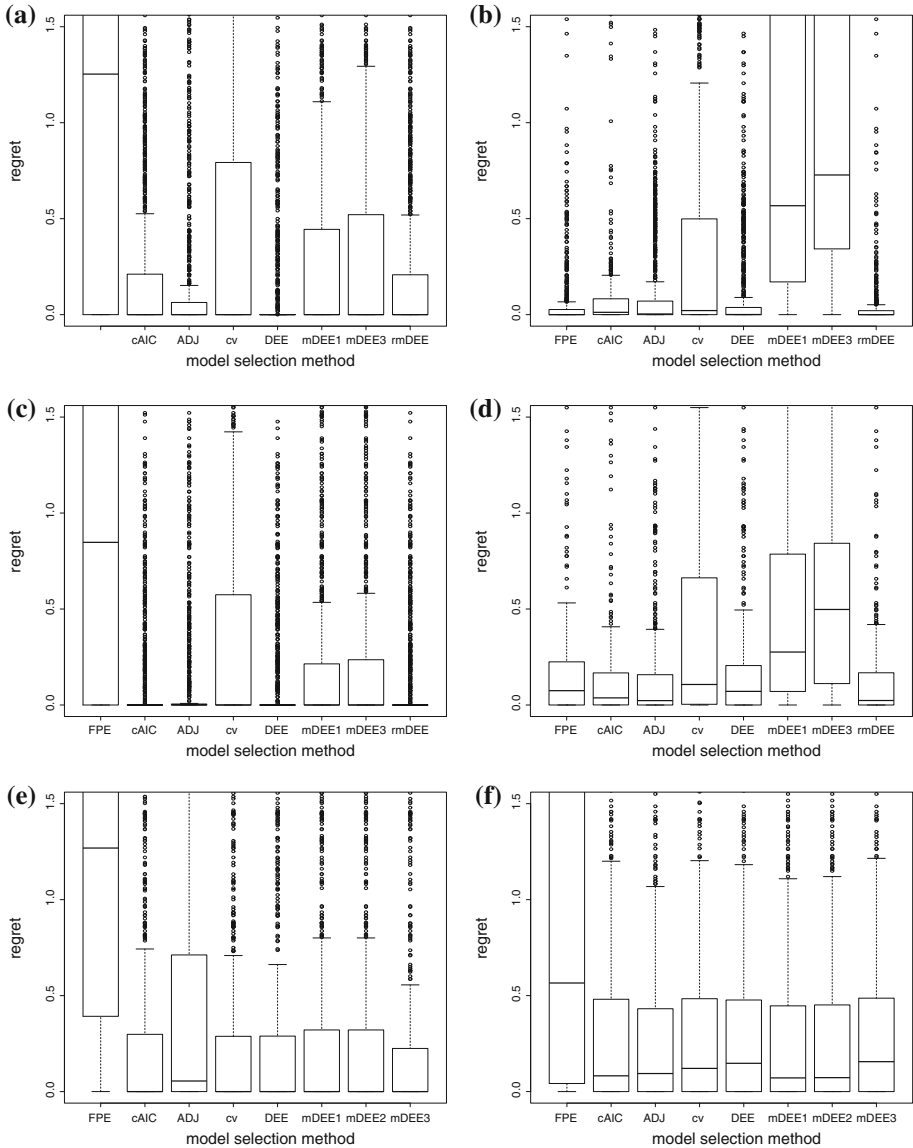
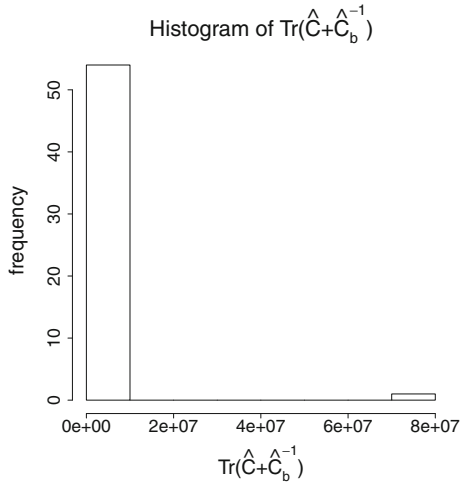


Fig. 2 Boxplot of regret for real-world data sets. **a** data: eheat, $n = 20$. **b** data: eheat, $n = 50$. **c** data: ecool, $n = 20$. **d** data: ecool, $n = 50$. **e** data: abalone, $n = 20$. **f** data: abalone, $n = 50$

worked significantly better than mDEE1 or mDEE3. On real-world data, mDEE1 slightly performed better than mDEE2 or mDEE3. However, their differences are little. In most cases, mDEE (or rmDEE) dominated DEE or at least performed equally. Remarkably, mDEE always dominated ADJ except ‘eheat’ when $n = 20$. As a whole, mDEE (or rmDEE) often performed the best or the second best.

Fig. 3 Histogram of the quantity $\text{Tr}(\hat{C}_+ \hat{C}_b^{-1})$ of mDEE3 when $n = 10$



7 Conclusion

Even though the idea of DEE seems to be promising, it was reported that DEE performs worse than ADJ which was the state-of-the-art. By checking the derivation of DEE, we found that the resultant form of DEE is valid in a sense but its derivation includes an inappropriate part. By refining the derivation in the generalized setting, we defined a class of valid risk estimators based on the idea of DEE and showed that more reasonable risk estimators could be found in that class.

Both DEE and mDEE assume that a large set of unlabeled data is available. Even though these unlabeled data can also be used to estimate the parameter (i.e., semi-supervised learning), DEE and mDEE do not use them for parameter estimation. Hence, combining the idea of DEE with semi-supervised estimator is an interesting future work. However, it seems not to be an easy task because the derivation of DEE strongly depends on the explicit form of LSE.

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