
Inverse Methods for Missing Data Imputation

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Abstract

Iterative imputation is a prevalent method for completing missing data, which involves iteratively imputing each feature by treating it as a target variable and predicting its missing values using the remaining features. However, existing iterative imputation methods exhibit two critical defects: (1) model misspecification, where a uniform parametric form of model is applied across different features, conflicting with heterogeneous data generation processes; (2) underuse of oracle features, where all features are treated as potentially missing, neglecting the valuable information in fully observed features. In this work, we propose kernel point imputation (KPI), a bi-level optimization framework designed to address these issues. The inner-level optimization optimizes the model form for each feature in a reproducing kernel Hilbert space, mitigating model misspecification. The outer-level optimization leverages oracle features as supervision signals to refine imputations. Extensive experiments on real-world datasets demonstrate that KPI consistently outperforms state-of-the-art imputation methods. Code is available at <https://github.com/FMLYD/kpi.git>.

1 Introduction

Missing data is a ubiquitous challenge in real-world data collection and analytics [24, 45]. For example, in manufacturing, temperature sensors may fail due to overheating or electrical disruptions, compromising data integrity and impeding analytical workflows [1]. Similarly, equipment-monitoring systems can experience lost connectivity in electrical sensors, impeding fault detection and introducing security risks [36]. These issues highlight the importance of missing data imputation (MDI) techniques, which aim to recover missing data using observed ones, thereby enhancing the integrity of collected datasets and the reliability of data-driven applications.

Existing MDI methods can be broadly categorized as discriminative or generative [5]. On the one hand, discriminative methods, such as statistical imputation (e.g., mean and median imputation [44]) and iterative imputation (which iteratively predicts missing values using univariate models [26, 29]), have been well developed. On the other hand, generative methods have recently attracted attention for their capacity to model complex data structures [1]. However, they often encounter training challenges [18, 25] or rely on strong data assumptions [42, 27]. Empirically, generative methods may

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frequently be outperformed by discriminative methods [45, 23]. Therefore, discriminative methods remain the preferred choice for MDI in practice [39].

Among discriminative methods, iterative imputation is widely adopted due to its straightforward implementation and strong empirical performance. It specifies univariate models for each feature conditioned on the rest and iteratively imputes missing values until convergence [26]. However, this approach has two limitations. First, it assumes that all features contain missing values, neglecting the utility of fully observed features, known as *oracle features*, which can provide strong supervisory signals for imputation. Second, it applies a fixed-form parametric model to all features, which risks model misspecification, as different features often exhibit heterogeneous dependencies that cannot be adequately captured by a fixed-form parametric model [5].

To counteract the two limitations, we reformulate iterative imputation as a bi-level optimization problem. The inner-level optimization adaptively selects functional forms from reproducing kernel Hilbert spaces (RKHS) for each feature, reducing model misspecification. The outer-level optimization aligns the imputed values with oracle features, leveraging them as direct supervision signals. Subsequently, we propose *kernel point imputation* (KPI), which expresses the optimal model as a linear combination of kernel functions, enabling efficient solution via stochastic gradient descent. Furthermore, we design an adaptive kernel ensemble strategy to dynamically combine kernels, thereby enhancing model expressiveness and alleviating hyperparameter selection challenge amidst incomplete data.

Contributions. The key contributions of this study are summarized as follows:

- We introduce a bi-level optimization framework for MDI which optimizes model form for each feature within a RKHS to address model misspecification and exploits oracle features as supervision to refine imputation results.
- We develop the KPI algorithm, which solves the bi-level optimization problem via stochastic gradient descent. Additionally, we develop a kernel ensemble method to counteract the difficulty of kernel parameter selection amidst missing data.
- We conduct extensive experiments to demonstrate the superiority of KPI over existing MDI methods and to highlight the utility of oracle features in enhancing imputation accuracy.

2 Preliminaries

As a preliminary note, this study aims to impute missing values as an *end* goal—specifically, to estimate their most probable values. We are not considering imputation as a means to obtain input for some downstream tasks [5], such as training regression models for label prediction [16, 14] or pseudo-labeling for unbiased learning [10]. Methods in these scenarios often require joint training to optimize specific objectives [16]. In this work, we concentrate on the MDI problem.

Suppose $\mathbf{X}^{(\text{id})} \in \mathbb{R}^{N \times D}$ is the ideally complete data matrix with N samples and D features. The presence of missing entries in $\mathbf{X}^{(\text{id})}$ is indicated by a binary matrix $\mathbf{M} \in \{0, 1\}^{N \times D}$, where each entry $M_{n,d}$ is set to 1 if the corresponding entry $\mathbf{X}_{n,d}^{(\text{id})}$ is missing, and 0 otherwise. Consequently, the observed dataset $\mathbf{X}^{(\text{obs})}$ can be derived using the Hadamard product:

$$\mathbf{X}^{(\text{obs})} := \mathbf{X}^{(\text{id})} \odot (1 - \mathbf{M}) + \text{nan} \odot \mathbf{M}. \quad (1)$$

The goal of MDI is to recover the missing entries by constructing an imputation matrix $\mathbf{X}^{(\text{imp})} \in \mathbb{R}^{N \times D}$ that closely approximates $\mathbf{X}^{(\text{id})}$. Different imputation methods vary in how they generate $\mathbf{X}^{(\text{imp})}$ from $\mathbf{X}^{(\text{obs})}$ and \mathbf{M} .

One prevalent approach is the iterative imputation method, which iteratively imputes each feature by treating it as a target variable and predicting its missing values using the remaining features as inputs. Specifically, in the training stage, let the d -th feature as the target feature, denoted as $\mathbf{Y}_d^{(\text{obs})} = \mathbf{X}_{:,d}^{(\text{obs})}$, the method fits an imputation model f_θ with parameters θ that learns the relationship between the target feature and the remaining features:

$$\min_{\theta} \left\| \mathbf{Y}_d^{(\text{obs})} - f_\theta(\mathbf{X}_{:,-d}^{(\text{obs})}) \right\|_2^2, \quad (2)$$

where $\mathbf{X}_{:,-d}^{(\text{obs})}$ denotes the matrix $\mathbf{X}^{(\text{obs})}$ with the d -th column removed. The method cycles the target feature for D times, training univariate imputation models for all features. In the inference stage,

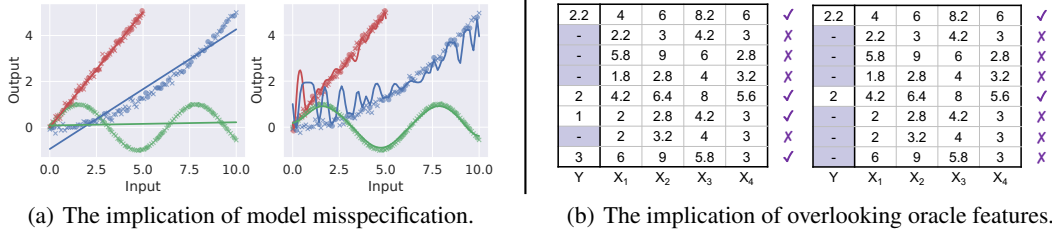


Figure 1: Case study illustrating the limitations of iterative imputation. In panel (a), circular and cross markers indicate observed and missing values, respectively, while lines represent imputation model outputs. In panel (b), “✓” denotes whether a sample can be used for training the imputation model for Y ; dark areas indicate missing indices in Y at missing ratios of 50% (left) and 75% (right).

imputation proceeds iteratively: for each target feature, its missing values are estimated using the corresponding univariate model, incorporating previously imputed values of other features. The imputed columns are concatenated to construct the imputation matrix $\mathbf{X}^{(\text{imp})}$.

3 Methodology

3.1 Motivation

Iterative imputation approaches MDI to a canonical regression problem, estimating each feature using the remaining features. In this section, we demonstrate that this approach leads to model misspecification and underuse of oracle features, thereby degrading imputation performance.

The first limitation is the risk of model misspecification. Iterative imputation methods typically employ a single predefined parametric form for all features, such as linear models [26] or decision trees [29]. However, real-world data often exhibit heterogeneous dependencies among features that cannot be effectively captured by a single parametric model [5]. For instance, temperature sensor data in a manufacturing process may have a linear relationship with pressure, while vibration data may display a nonlinear relationship with pressure. Imposing a uniform parametric form thus fails to accommodate these diverse dependencies, leading to suboptimal imputation performance.

The second limitation is the underuse of oracle features. Iterative methods, by treating all features as equally prone to missingness, suffer from limited training data under high missing ratios. Oracle features, which have minimal missing values, can provide critical supervision for imputing other variables. For instance, in health records, demographic data often serves as reliable oracle features, while in industrial settings, catastrophic data can fulfill this role. However, iterative approaches neglect these reliable features, thereby limiting overall imputation quality.

Case study. To illustrate the above limitations of the existing iterative imputation method, a case study is conducted. Fig. 1 (a) demonstrates how a fixed model form can lead to model misspecification. In the left panel, a linear model accurately captures the linear feature (red) but fails to fit the nonlinear features (blue and green). Conversely, the right panel shows that a nonlinear model fits the sine feature well but overfits the other features. Therefore, a fixed parametric form risks misspecification and thereby hampers imputation performance. Fig. 1 (b) illustrates the impact of overlooking oracle features. To impute missing values in the target column Y , the iterative method constructs a univariate model using X_1, \dots, X_4 as inputs. The model is trained using solely samples with non-missing Y values. With high missing ratios, only a few samples are usable for training (two in the right panel), which is insufficient to learn a robust model. In contrast, the four fully observed oracle features (X_1, \dots, X_4) are overlooked, forfeiting an opportunity to enhance imputation accuracy.

These limitations underscore the need for an improved iterative approach that effectively leverages oracle features and mitigates model misspecification for improved imputation performance. In particular, there are three key questions to be explored: (1) How to adaptively elect different model forms to each feature to reduce misspecification? (2) How to incorporate oracle features in imputation? (3) Do model-form adaptation and oracle features indeed boost imputation accuracy?

3.2 A bi-level optimization framework for iterative imputation

We propose a novel bi-level optimization formulation to overcome the limitations of iterative methods. This framework customizes model forms for each feature within a reproducing kernel Hilbert space (RKHS) and integrates oracle features as supervision signals.

Based on the iterative imputation in (2), to mitigate model misspecification, we replace the single parametric form of the standard iterative approach, expressed as the f_θ in (2), with a flexible form in RKHS. Given the d -th feature as the target: $\mathbf{Y}^{(\text{obs})} = \mathbf{X}_{:,d}^{(\text{obs})}$, we reformulate the imputation task as:

$$f^* = \arg \min_{f \in \mathcal{H}} \left\| \mathbf{Y}^{(\text{obs})} - f(\mathbf{X}_{:,-d}^{(\text{obs})}) \right\|_2^2 + \lambda \|f\|_{\mathcal{H}}^2, \quad (3)$$

where f^* is the optimal model for that feature. The capacity of RKHS ensures that f^* can capture effectively heterogeneous feature relationships, reducing the risk of misspecification.

To exploit oracle features, a natural approach is to incorporate them as supervision signals that guide imputation. Suppose $\mathbf{Y}^{(\text{obs})}$ is an oracle feature and f^* is the associated optimum estimator; we update the imputed values as:

$$\min_{\mathbf{X}^{(\text{miss})}} \left\| \mathbf{Y}^{(\text{obs})} - f^*(\mathbf{X}_{:,-d}^{(\text{miss})}, \mathbf{X}_{:,-d}^{(\text{obs})}) \right\|_2^2. \quad (4)$$

This approach is based on a perhaps surprising point-of-view: if $\mathbf{X}^{(\text{miss})}$ is well-imputed, applying f^* should yield outputs consistent with the ground truth. Otherwise, the imputations of $\mathbf{X}^{(\text{miss})}$ deviate from the underlying relationship captured by f^* . Thus, by adjusting $\mathbf{X}^{(\text{miss})}$ to minimize this discrepancy, the imputation process self-corrects, effectively using oracle features as a supervision mechanism.

Combining (3) and (4) yields our bi-level optimization framework for MDI. Given the d -th feature as the target, *i.e.*, $\mathbf{Y}^{(\text{obs})} = \mathbf{X}_d^{(\text{obs})}$, $\mathbf{X} = (\mathbf{X}_{:,-d}^{(\text{miss})}, \mathbf{X}_{:,-d}^{(\text{obs})})$, the optimization problem is formulated as:

$$\min_{\mathbf{X}^{(\text{miss})}} \min_{f \in \mathcal{H}} \left\| \mathbf{Y}^{(\text{obs})} - f(\mathbf{X}) \right\|_2^2 + \lambda \|f\|_{\mathcal{H}}^2. \quad (5)$$

Similar to the standard iterative method, each feature—*both* oracle features and those with missing values—is iteratively treated as the target feature $\mathbf{Y}^{(\text{obs})}$. In the inner optimization, the optimal function f is selected within the RKHS, thereby mitigating model misspecification. In the outer optimization, the imputed values are refined, effectively incorporating oracle features as supervision signals. Therefore, this bi-level optimization framework provides a principled approach to MDI, addressing the limitations of iterative methods.

3.3 Kernel function, universal property and learning objective

To solve the inner loop in (5), we approximate the optimum function f^* by leveraging Gaussian kernels in the RKHS. We start by clarifying key kernel properties in Definition 3.1 and 3.2.

Definition 3.1 (Kernel function). Let \mathcal{X} be a non-empty set. A function $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is a kernel function if there exists a Hilbert space \mathcal{H} and a feature map $\psi : \mathcal{X} \rightarrow \mathcal{H}$ such that $\forall x, x' \in \mathcal{X}$, $K(x, x') := \langle \psi(x), \psi(x') \rangle_{\mathcal{H}}$.

Definition 3.2 (Universal kernel). For \mathcal{X} compact Hausdorff, A universal kernel ensures that any continuous function $e : \mathcal{X} \rightarrow \mathbb{R}$ can be approximated arbitrarily well within RKHS \mathcal{H} . Specifically, for any $\epsilon > 0$, there exists $f \in \mathcal{H}$ such that: $\sup_{x \in \mathcal{X}} |f(x) - e(x)| \leq \epsilon$.

Gaussian kernel is a typical kernel function formulated as:

$$K(x, x') = \exp \left(-\frac{\|x - x'\|^2}{2\sigma^2} \right),$$

which satisfies the universal property in Definition 3.2 [28]. It implies that by using the Gaussian kernel, the associated RKHS $\mathcal{H} = \text{span}\{K(\cdot, x) \mid x \in \mathcal{X}\}$ admits uniform approximation of any continuous function.

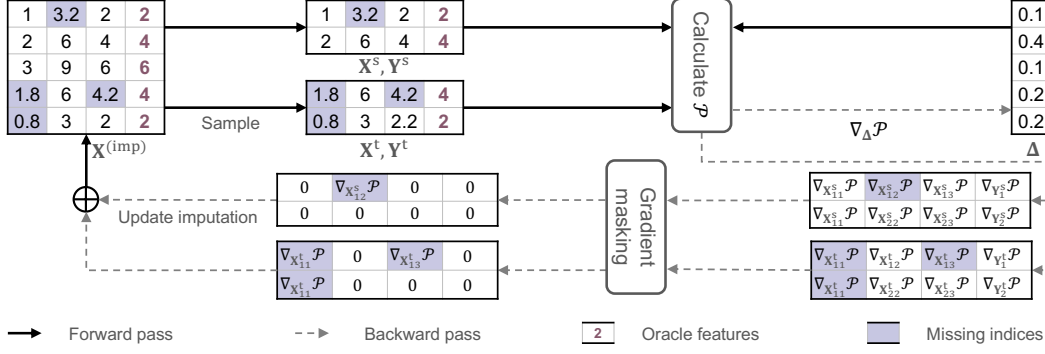


Figure 2: Visualization of the workflow of KPI, where the dataset contains 5 samples and 4 features. The sampling batch size is set to 2. The last column is the oracle feature without missing values.

Lemma 3.3 (Representer theorem). *Suppose $h(\|f\|) : \mathbb{R}_+ \rightarrow \mathbb{R}$ is a non-decreasing function. The minimizer of an empirical risk functional regularized by $h(\|f\|)$ admits the form: $f^*(\cdot) = \sum_{i=1}^n \alpha_i K(\cdot, x_i)$ where $\alpha = (\alpha_1, \dots, \alpha_n)^\top$ and K is the associated kernel function.*

Lemma 3.4. *Let $Y^s, Y^t \in \mathbb{R}^{B \times 1}$ be the target feature and X^s, X^t be the corresponding input features; Suppose f^* is the optimal model minimizing the empirical risk in the inner optimization of (5), its output on X^t is given by $f^*(X^t) = K_{X^t X^s} \cdot \alpha$, where $\alpha = (K + \lambda I)^{-1} Y^s$; $K_{X^t X^s}$ is the kernel matrix computed with X^t and X^s .*

Since \mathcal{H} is potentially infinite-dimensional, directly identifying f^* is infeasible. Nevertheless, the representer theorem in Lemma 3.3 provides a finite approximation to f^* . Accordingly, by sampling two batches of data—target features (Y^s, Y^t) and input features (X^s, X^t)—Lemma 3.4 yields that the output of f^* at X^t can be represented as:

$$f^*(X^t) = K_{X^t X^s} (K_{X^s X^s} + \lambda I)^{-1} Y^s, \quad (6)$$

which analytically expresses the output of the optimum model f^* as a linear combination of kernel functions. It enables adaptively selecting the optimum model for each feature, and simplifies the bi-level optimization problem in (5) to a differentiable loss function:

$$\min_{X^s, X^t} \|Y^t - K_{X^t X^s} (K_{X^s X^s} + \lambda I)^{-1} Y^s\|_2^2, \quad (7)$$

Furthermore, selecting kernel hyperparameters (e.g., Gaussian kernel variance) can be challenging amidst missing data. To alleviate this problem, we introduce multiple kernels with distinct parameters and learn to ensemble them adaptively. Suppose K^1, K^2, \dots, K^E are E kernel matrices, each with a different configuration. We define a learnable simplex vector $\Delta \in \mathbb{R}^E$, and construct the ensembled kernel as $K^\Delta = K^1 \Delta_1 + \dots + K^E \Delta_E$. Putting together, the final objective becomes:

$$\mathcal{P} = \|Y^t - K_{X^t X^s}^\Delta (K_{X^s X^s}^\Delta + \lambda I)^{-1} Y^s\|_2^2. \quad (8)$$

3.4 Overall workflow

While the learning objective is well defined, its role in actual imputation remains unclear. To this end, we propose the kernel point imputation (KPI) method, which iteratively minimizes the objective (8) to refine missing value imputations. The core procedure is shown in Fig. 2 and detailed as follows.

Initialization. Given the incomplete dataset $X^{(obs)}$, we initialize missing entries using the mean of observed steps, obtaining an initial imputation matrix X^{imp} . The imputed values are treated as learnable parameters, and their gradients are tracked throughout training.

Forward Pass. Two batches are sampled from the imputation matrix. In each iteration, a column is randomly chosen as the target feature ($Y^s, Y^t \in \mathbb{R}^{B \times 1}$), with the remaining columns as input features ($X^s, X^t \in \mathbb{R}^{B \times (D-1)}$), where B represents batch size, s and t differentiates different batches. The objective \mathcal{P} is computed following (8).

Table 1: Imputation performance in terms of MSE and MAE on 7 datasets.

Datasets	BT		CC		CBV		IS		PK		QB		WQW	
Metrics	MSE	MAE	MSE	MAE	MSE	MAE	MSE	MAE	MSE	MAE	MSE	MAE	MSE	MAE
Mean	0.742	0.452	0.837	0.789	0.829	1.165	0.754	4.145	0.740	2.841	0.589	4.682	0.764	1.121
Mode	0.948	0.770	0.935	1.159	1.026	1.749	0.925	7.741	1.254	7.832	0.593	6.240	0.823	1.372
Median	0.706	0.469	0.811	0.884	0.820	1.165	0.713	4.356	0.698	3.029	0.500	5.066	0.756	1.123
MICE	0.580	0.127	0.745	0.474	0.856	1.021	0.733	4.539	0.417	1.312	0.536	3.415	0.824	0.971
Miss.F	0.560	0.241	0.732	0.650	0.764	0.994	0.593	3.277	0.526	1.497	0.436	3.202	0.686	0.898
Sinkhorn	0.835	0.466	0.906	0.796	0.898	1.225	0.848	4.945	0.827	3.233	0.775	6.114	0.857	1.170
TDM	0.730	0.487	0.819	0.769	0.799	1.113	0.726	3.965	0.722	2.792	0.570	4.756	0.752	1.098
CSDI-T	0.726	1.870	0.849	2.683	0.821	3.802	0.761	15.493	0.731	12.291	0.575	19.919	0.780	4.084
MissDiff	0.719	1.332	0.840	1.699	0.816	3.523	0.749	13.432	0.728	14.462	0.564	23.320	0.758	5.184
GAIN	0.730	0.396	0.777	0.688	0.729	0.942	0.572	3.318	0.448	1.413	0.476	4.669	0.754	1.095
MIRACLE	0.795	0.674	0.487	0.305	0.831	1.154	3.208	45.816	3.518	36.784	0.521	3.975	0.555	0.685
MIWAE	0.582	0.266	0.746	0.630	0.807	1.071	0.636	4.118	0.525	1.804	0.475	4.977	0.657	0.844
Remasker	0.439	0.131	0.767	0.750	0.528	0.522	0.599	3.584	0.447	1.268	0.401	2.811	0.546	0.636
NewImp	0.465	0.177	0.412	0.292	0.405	0.401	0.431	2.495	0.320	0.8575	0.332	2.992	0.497	0.692
kpi(Ours)	0.397	0.121	0.347	0.284	0.402	0.394	0.400	2.387	0.319	0.747	0.264	2.131	0.491	0.685

Note: Each entry represents the average results at four missing ratios: 0.1, 0.2, 0.3, and 0.4. The best and second-best results are **bolded** and [underlined](#), respectively.

Backward Pass. The gradients of \mathcal{P} with respect to \mathbf{X}^s , \mathbf{X}^t and Δ are calculated using automatic differentiation. The imputed values in \mathbf{X}^s and \mathbf{X}^t as well as Δ are then updated using gradient descent with an update rate η :

$$\begin{aligned}
\mathbf{X}^s &\leftarrow \mathbf{X}^s - \eta \nabla_{\mathbf{X}^s} \mathcal{P} \odot \mathbf{M}^s, \\
\mathbf{X}^t &\leftarrow \mathbf{X}^t - \eta \nabla_{\mathbf{X}^t} \mathcal{P} \odot \mathbf{M}^t, \\
\Delta &\leftarrow \Delta - \eta \nabla_{\Delta} \mathcal{P},
\end{aligned} \tag{9}$$

where only the missing values (with $\mathbf{M} = 1$) are updated, while the observed values (with $\mathbf{M} = 0$) remain unchanged during this process. Moreover, the gradient of the matrix inverse term is stopped for numerical stability. KPI iteratively executes the forward and backward passes sampling different batches until hitting the early-stopping criteria on the validation dataset. In this process, each feature is iteratively treated as the target feature while the remaining features are treated as the input features. This ensures that all features—including oracle features—are fully exploited as supervision signals.

4 Empirical Investigation

4.1 Experimental setup

- **Datasets:** The empirical study is performed on public tabular datasets from [1], including Blood Transfusion(BT) Concrete Compression (CC) Connectionist Bench Vowel (CBV) Ionosphere (IS) Parkinsons (PS) Qsar Biodegradation (QB) Wine Quality White (WQW). To simulate missing data scenarios, we employ a mask matrix generated by a Bernoulli random variable with a preset mean.
- **Baselines:** The performance of KPI is compared against various imputation methods, including iterative imputers (MICE [26], Miss.F. [29]), and generative models (GAIN [42], MIWAE [19], Miss.D [24], CSDI-T [31], ReMasker [2], and NewImp [1]). We also assess methods that do not conform to these categories, such as MIRACLE [7], Sinkhorn [23], and TDM [45].
- **Implementation details:** To ensure convergence, we cap the number of iterations at 500 and adopt an early stopping criterion based on validation performance, with a patience of 10 epochs. The Adam optimizer is used for training [6]. Key hyperparameters, namely η and B, are determined by allocating 5% of the training data for validation and finetuning over [0.0001, 0.01] for η and

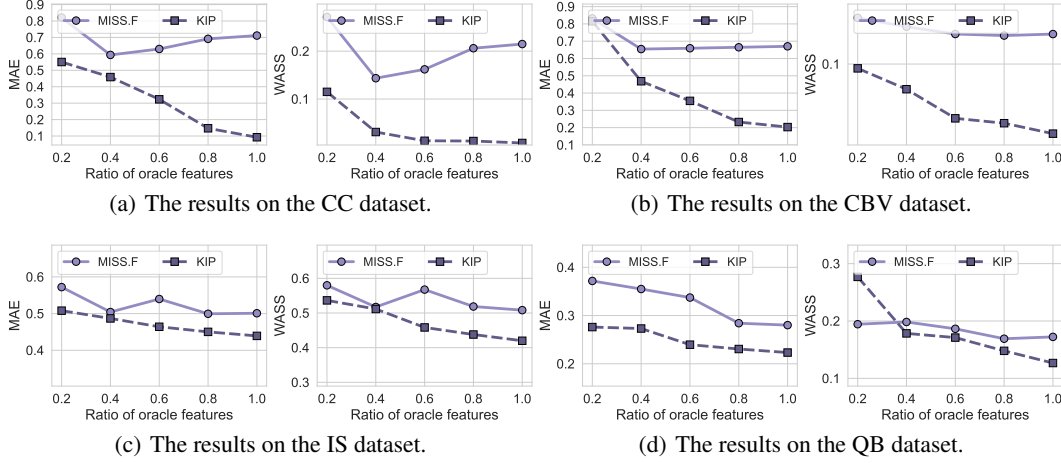


Figure 3: The performance of Miss.F and KPI given varying ratios of oracle features.

[64, 512] for B. Performance is assessed using modified mean absolute error (MAE) and mean squared error (MSE), focusing on the imputed values at missing entries, following [45, 5]. In addition, we report the distribution discrepancy (WASS), measured as the Wasserstein distance [5]. The experiments are performed on a platform with two Intel(R) Xeon(R) Platinum 8383C CPUs @ 2.70GHz and a NVIDIA GeForce RTX 4090 GPU.

4.2 Overall performance

Tab. 1 presents the average imputation results of KPI and baseline methods under missing ratios $p_{\text{miss}} = 0.1, 0.2, 0.3, \text{ and } 0.4$. Key observations are summarized as follows:

- The iterative imputers exhibits promising performance in most cases. For instance, MICE outperforms simple imputers by large margin over most datasets. MissForest employs random forest as the base model, excelling in handling tabular data, which further improves imputation quality.
- The canonical generative imputers [31, 24], originally tailored for time-series data, often falling behind iterative methods. This can be attributed to the implicit maximization of imputation entropy in diffusion models, which negatively impacts accuracy [1]. By contrast, recent generative approaches such as NewImp and Remasker handle this issue and achieve strong results, obtaining the best results among baseline methods.
- KPI improves the iterative imputers by adaptively selecting the optimal imputer for each feature and involving oracle features as supervision signals. This strategy consistently improves performance, as evidenced by KPI outperforming all baselines across all 7 datasets—often by a substantial margin, particularly on the CC and QB datasets—demonstrating strong practical effectiveness.

4.3 Impact of oracle features

In this section, we assess the impact of using oracle features as supervision signal on imputation performance. Specifically, we simulate based on complete datasets to generate varying ratios of oracle features and evaluate the imputation performance. Two models are considered: KPI and another canonical iterative imputer: Miss.F.

The results are presented in Fig. 3. As the ratio of oracle features increases, KPI consistently exhibits lower imputation error, showcasing the utility of oracle features. In contrast, Miss.F shows little improvement as oracle feature ratio increases. This difference arises because Miss.F only uses oracle features as inputs, whereas KPI exploits them as supervision signals to refine the imputation results.

Table 2: Varying kernel number results.

CC						
E	MSE	Δ MSE	WASS	Δ WASS	MAE	Δ MAE
1	0.082	-	0.058	-	0.155	-
3	0.070	14.6%↓	0.055	5.2%↓	0.116	25.2%↓
5	0.069	15.9%↓	0.046	20.7%↓	0.108	30.3%↓
7	0.065	20.7%↓	0.039	32.8%↓	0.091	41.3%↓

CBV						
E	MSE	Δ MSE	WASS	Δ WASS	MAE	Δ MAE
1	0.128	-	0.095	-	0.233	-
3	0.110	14.1%↓	0.085	10.5%↓	0.226	3.0%↓
5	0.098	23.4%↓	0.075	21.1%↓	0.216	7.3%↓
7	0.087	32.0%↓	0.066	30.5%↓	0.205	12.0%↓

BT						
Distances	MSE	Δ MSE	WASS	Δ WASS	MAE	Δ MAE
1	0.334	-	0.109	-	0.363	-
3	0.318	4.8%↓	0.101	7.3%↓	0.352	3.0%↓
5	0.305	8.7%↓	0.096	11.9%↓	0.343	5.5%↓
7	0.302	9.6%↓	0.089	18.3%↓	0.338	6.9%↓

Table 3: Varying kernel function results.

CC						
Kernel	MSE	Δ MSE	WASS	Δ WASS	MAE	Δ MAE
Linear	0.099	-	0.051	-	0.203	-
Poly	0.065	34.3%↓	0.039	23.5%↓	0.091	55.2%↓
Laplacian	0.068	31.3%↓	0.042	17.6%↓	0.093	54.2%↓
Gaussian	0.076	23.2%↓	0.035	31.4%↓	0.082	59.6%↓

CBV						
Kernel	MSE	Δ MSE	WASS	Δ WASS	MAE	Δ MAE
Linear	0.089	-	0.087	-	0.219	-
Poly	0.087	2.2%↓	0.088	1.1%↑	0.214	2.3%↓
Laplacian	0.083	6.7%↓	0.080	8.1%↓	0.211	3.7%↓
Gaussian	0.087	2.2%↓	0.066	24.1%↓	0.205	6.4%↓

BT						
Distances	MSE	Δ MSE	WASS	Δ WASS	MAE	Δ MAE
Linear	0.326	-	0.101	-	0.359	-
Poly	0.305	6.4%↓	0.090	10.9%↓	0.342	4.7%↓
Laplacian	0.316	3.1%↓	0.091	9.9%↓	0.346	3.6%↓
Gaussian	0.302	7.4%↓	0.089	11.9%↓	0.338	5.8%↓

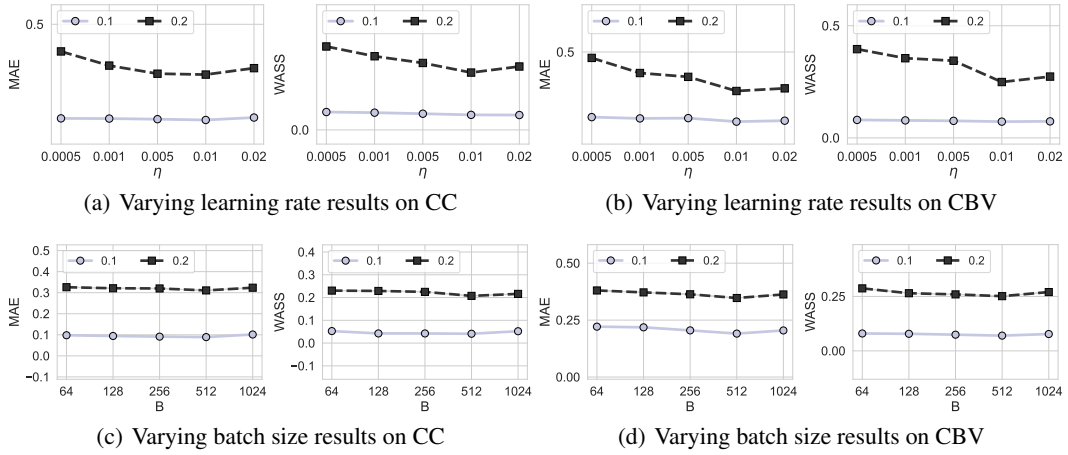


Figure 4: Varying learning rate and batch size results with missing ratios 0.1 and 0.2.

4.4 Impact of kernel strategy

In this section, we analyze the impact of kernel function and kernel amount (E) on imputation performance. The key observations are summarized as follows.

- The multiple kernel ensembling mechanism has a substantial impact. As shown in Tab. 2, increasing E from 1 to 7 consistently reduces MSE from 0.082 to 0.065, indicating a relative reduction of 20.7%. This gain is attributed to the increased flexibility in adaptively selecting kernel parameters, allowing KPI to better represent the optimal imputation model for each feature.
- The performance of different kernel functions showcases the importance of kernel universality. The linear kernel, which is not universal and has limited RKHS capacity, yields the worst performance. The polynomial kernel, with a larger RKHS, performs better. The Gaussian kernel exhibits the best overall performance. The superiority is attributed to its universality, i.e., the associated RKHS admits uniform approximation of any continuous function. Such extensive RKHS capacity enables KPI to optimize the imputation model for each feature, thereby enhancing imputation performance.

4.5 Parameter sensitivity analysis

In this section, we examine the influence of critical hyperparameters on the performance of KPI in Fig. 4. Below are the key observations:

- The update rate (η) plays a pivotal role in controlling the volume of updates to the imputation matrix each epoch. As η is reduced from 0.02 to approximately 0.01, both MAE and RMSE decrease, indicating that a smaller η enhances update stability. However, further reduction of η to 0.001 results in increased MAE and RMSE, where the meaningful update direction becomes overshadowed by noise, preventing model convergence within the allocated epochs.
- The batch size (B) affects the scale of the problem in calculating discrepancies, with sizes ranging from 64 to 1024 examined. There is a weak yet consistent decrease in MAE and RMSE as the batch size increases to $B = 512$, enhancing the reliability of estimations. Increasing the batch size beyond this point yields diminishing returns and may lead to unnecessary computational overhead.

5 Related works

The pervasive presence of missing data undermines the integrity of collected datasets and the reliability of data-driven applications, underscoring the necessity for effective missing data imputation (MDI). To achieve accurate MDI, existing approaches can be broadly categorized into two paradigms: discriminative and generative, each with distinct advantages and limitations [5, 21].

The iterative method [29, 26, 43, 15] is one of the most popular methods in discriminative imputation, initiated from imputation by chained equations (ICE) [26], which employs specific models to estimate missing values for each feature based on the remaining observable features. On the basis of ICE, a line of work advocates for employing modern parametric models, such as neural networks [19, 7], Bayesian models [26] and random forest [29], which enhances the capacity of imputation models and thereby accommodating complex missing patterns. In a different line of work, various training techniques are investigated within the paradigm, such as multiple imputation [26], ensemble learning [29], and multitask learning [19], which enhances the utility to accommodate diverse contexts. While this paradigm offers enhanced flexibility and accuracy, it fails to utilize the oracle features effectively and risks model misspecification, which can lead to suboptimal imputation results in noisy environments. Our research advances this methodology by handling the two limitations.

Apart from the iterative methods, there are other notable approaches in the discriminative paradigm. The simple direct paradigm employs elementary statistical measures like mean, median, and mode to replace missing values, offering quick and straightforward solutions. However, this approach lacks the capacity to accommodate complex relationships [17, 20], often producing trivial and inadequate imputation results that fail to meet the expectation in practice. Another notable approach is matrix factorization, which decomposes the data matrix into two low-rank matrices, capturing the latent structure of the data for imputation [8, 4]. This method is particularly effective in collaborative filtering and recommendation systems [12, 37]. Recent advances explore a novel methodology based on distribution discrepancy minimization [45, 23]. This approach builds on the assumption that, under the independent and identically distributed (i.i.d.) condition, any two data batches should share the same underlying distribution, thereby exhibiting minimal discrepancy. Subsequent studies have extended this idea by refining discrepancy measures to accommodate different data characteristics such as neighboring effects [40, 35], noisy observations [36], and temporal dependencies [39].

The generative paradigm restates imputation as a conditional generation problem, using advanced neural architectures and generative training strategies, such as generative adversarial networks [42, 30, 13] and diffusions [31, 41, 1], to approximate data distributions and perform imputation. This strategy incorporates the strengths of generative models, capturing and utilizing complex relationships, which potentially enhances the imputation quality when ample data is available. However, it also bears the defects with generative models, such as the instability associated with adversarial training and the operational complexity of diffusions [18, 25], hampering their use in practice.

6 Conclusion

Iterative imputation methods are widely used for handling missing data, yet existing approaches are often limited by model misspecification and underuse of oracle features. To overcome these challenges, we introduce KPI, a bi-level optimization framework which optimizes model form within RKHS for each feature, reducing model misspecification, and exploits oracle features as effective supervision. Extensive experiments on real-world datasets demonstrate that KPI achieves superior imputation performance and effectively leverages oracle features.

Limitations & future work. In this work, we do not accommodate potential noise in datasets, which is a prevalent challenge in industrial settings [4, 3]. Future research could incorporate robust optimization techniques and truncate outliers in the kernel matrix which has potential to improve noise robustness. Additionally, this work mitigates the difficulty of concise kernel parameter selection via adaptive ensembling, which is an heuristic approach. Subsequent work may explore meta-learning strategies with theoretical guarantees for accurate kernel parameter selection.

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A Theoretical justification

Building upon the foundational theorems established earlier, we delve deeper into the theoretical aspects of our kernel ridge regression-based imputation framework. By leveraging advanced properties of kernel functions—such as universality, injective mappings, and the reproducing property—we further substantiate the advantages and robustness of our method. This section introduces additional theorems and proofs that highlight these properties and their implications for the imputation problem.

Lemma A.1 (Representer theorem). *Suppose $h(\|f\|) : \mathbb{R}_+ \rightarrow \mathbb{R}$ is a non-decreasing function. The minimizer of an empirical risk functional regularized by $h(\|f\|)$ admits the form: $f^*(\cdot) = \sum_{i=1}^n \alpha_i K(\cdot, x_i)$ where $\alpha = (\alpha_1, \dots, \alpha_n)^\top$ and K is the associated kernel function.*

Proof. The proof can be found in Theorem 6.11 of Mohri et al. [22]. \square

Theorem A.2 (Lemma 3.4 in the main text). *Let $\mathbf{Y}^s, \mathbf{Y}^t \in \mathbb{R}^{B \times 1}$ be the target feature and $\mathbf{X}^s, \mathbf{X}^t$ be the corresponding input features; Suppose f^* is the optimal model minimizing the empirical risk in the inner optimization of (5), its output on \mathbf{X}^t is given by $f^*(\mathbf{X}^t) = \mathbf{K}_{\mathbf{X}^t \mathbf{X}^s} \cdot \alpha$, where $\alpha = (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{y}$; $\mathbf{K}_{\mathbf{X}^t \mathbf{X}^s}$ is the kernel matrix computed with \mathbf{X}^t and \mathbf{X}^s .*

Proof. Consider the samples \mathbf{X}^s and \mathbf{Y}^s where \mathbf{Y}^s is the observed target, and \mathbf{X}^s comprises the input features. The empirical risk minimization objective with ℓ_2 regularization to select the optimal functional form is

$$\min_{f \in \mathcal{H}} \|\mathbf{Y}^s - f(\mathbf{X}^s)\|_2^2 + \lambda \|f\|_{\mathcal{H}}^2, \quad (10)$$

which corresponds precisely to the inner loop of (5). According to Lemma A.1, when h is an identity function (in (10)) and \mathcal{H} is a RKHS associated with kernel K , the minimizer f^* must admit the explicit form

$$f^*(x) = \sum_{i=1}^B \alpha_i K(x, x_i^s), \quad (11)$$

for some coefficients $\alpha_1, \dots, \alpha_B$.

Substituting this form into the empirical risk (10), the optimization problem becomes

$$\min_{\alpha \in \mathbb{R}^B} \|\mathbf{Y}^s - \mathbf{K}_{\mathbf{X}^s \mathbf{X}^s} \alpha\|_2^2 + \lambda \alpha^\top \mathbf{K}_{\mathbf{X}^s \mathbf{X}^s} \alpha, \quad (12)$$

where $\mathbf{K}_{\mathbf{X}^s \mathbf{X}^s}$ is the $B \times B$ Gram matrix, with (i, j) -th entry $K(x_i^s, x_j^s)$, \mathbf{Y}^s is the length- B target vector, and α is the vector of coefficients.

Expanding the loss function in matrix notation yields

$$(\mathbf{Y}^s - \mathbf{K}_{\mathbf{X}^s \mathbf{X}^s} \alpha)^\top (\mathbf{Y}^s - \mathbf{K}_{\mathbf{X}^s \mathbf{X}^s} \alpha) + \lambda \alpha^\top \mathbf{K}_{\mathbf{X}^s \mathbf{X}^s} \alpha. \quad (13)$$

Due to symmetry of $\mathbf{K}_{\mathbf{X}^s \mathbf{X}^s}$, this simplifies to

$$\mathbf{Y}^{s\top} \mathbf{Y}^s - 2 \mathbf{Y}^{s\top} \mathbf{K}_{\mathbf{X}^s \mathbf{X}^s} \alpha + \alpha^\top (\mathbf{K}_{\mathbf{X}^s \mathbf{X}^s}^2 + \lambda \mathbf{K}_{\mathbf{X}^s \mathbf{X}^s}) \alpha. \quad (14)$$

According to the first-order condition, setting the derivative with respect to α to zero and solving for α gives

$$-2 \mathbf{K}_{\mathbf{X}^s \mathbf{X}^s}^\top \mathbf{Y}^s + 2 (\mathbf{K}_{\mathbf{X}^s \mathbf{X}^s}^2 + \lambda \mathbf{K}_{\mathbf{X}^s \mathbf{X}^s}) \alpha = 0, \quad (15)$$

which is equivalent to:

$$\mathbf{K}_{\mathbf{X}^s \mathbf{X}^s} (\mathbf{K}_{\mathbf{X}^s \mathbf{X}^s} + \lambda \mathbf{I}) \alpha = \mathbf{K}_{\mathbf{X}^s \mathbf{X}^s} \mathbf{Y}^s. \quad (16)$$

Assuming $\mathbf{K}_{\mathbf{X}^s \mathbf{X}^s}$ is invertible, we have:

$$(\mathbf{K}_{\mathbf{X}^s \mathbf{X}^s} + \lambda \mathbf{I}) \alpha = \mathbf{Y}^s. \quad (17)$$

which immediately follows from multiplying both sides by $\mathbf{K}_{\mathbf{X}^s \mathbf{X}^s}^{-1}$. Solving for α gives:

$$\alpha = (\mathbf{K}_{\mathbf{X}^s \mathbf{X}^s} + \lambda \mathbf{I})^{-1} \mathbf{Y}^s. \quad (18)$$

Substituting (18) into (11) leads to

$$f^*(x) = \sum_{i=1}^B \alpha_i K(x, x_i^s) = \mathbf{K}(x)(\mathbf{K}_{\mathbf{X}^s \mathbf{X}^s} + \lambda \mathbf{I})^{-1} \mathbf{Y}^s, \quad (19)$$

where $\mathbf{K}(x)$ is the $1 \times B$ vector $[K(x, x_1^s), \dots, K(x, x_B^s)]$. For a (possibly distinct) batch of inputs \mathbf{X}^t , evaluating f^* at each x_j^t gives

$$\begin{aligned} f^*(x_1^t) &= \sum_{i=1}^B \alpha_i K(x_1^t, x_i^s) = [K(x_1^t, x_1^s), K(x_1^t, x_2^s), \dots, K(x_1^t, x_B^s)] (\mathbf{K}_{\mathbf{X}^s \mathbf{X}^s} + \lambda \mathbf{I})^{-1} \mathbf{Y}^s, \\ f^*(x_2^t) &= \sum_{i=1}^B \alpha_i K(x_2^t, x_i^s) = [K(x_2^t, x_1^s), K(x_2^t, x_2^s), \dots, K(x_2^t, x_B^s)] (\mathbf{K}_{\mathbf{X}^s \mathbf{X}^s} + \lambda \mathbf{I})^{-1} \mathbf{Y}^s, \\ &\dots \\ f^*(x_B^t) &= \sum_{i=1}^B \alpha_i K(x_B^t, x_i^s) = [K(x_B^t, x_1^s), K(x_B^t, x_2^s), \dots, K(x_B^t, x_B^s)] (\mathbf{K}_{\mathbf{X}^s \mathbf{X}^s} + \lambda \mathbf{I})^{-1} \mathbf{Y}^s, \end{aligned} \quad (20)$$

which may be stacked to give the vector-valued expression

$$f^*(\mathbf{X}^t) = \mathbf{K}_{\mathbf{X}^t \mathbf{X}^s} (\mathbf{K}_{\mathbf{X}^s \mathbf{X}^s} + \lambda \mathbf{I})^{-1} \mathbf{Y}^s, \quad (21)$$

where $\mathbf{K}_{\mathbf{X}^t \mathbf{X}^s}$ is the matrix with entries $[\mathbf{K}_{\mathbf{X}^t \mathbf{X}^s}]_{ij} = K(x_i^t, x_j^s)$. The proof is completed. \square

Definition A.3 (Kernel Functions). Let $\mathbf{x}, \mathbf{x}' \in \mathbb{R}^D$ be two vectors in the input feature space. A *kernel function* $K : \mathbb{R}^D \times \mathbb{R}^D \rightarrow \mathbb{R}$ is a symmetric, positive semi-definite function that quantifies the similarity between \mathbf{x} and \mathbf{x}' . Commonly used kernel functions include:

1. **Linear Kernel:** $K_{\text{linear}}(\mathbf{x}, \mathbf{x}') = \mathbf{x}^\top \mathbf{x}'$, which computes the inner product between two vectors and corresponds to the case where no explicit feature transformation is applied.
2. **Polynomial Kernel:** $K_{\text{poly}}(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^\top \mathbf{x}' + c)^d$, where $c \geq 0$ is a constant coefficient trading off the influence of higher-order versus lower-order terms, and $d \in \mathbb{N}$ is the degree of the polynomial. It enables learning non-linear relationships by implicitly mapping the input features into a higher-dimensional polynomial feature space.
3. **Gaussian Kernel:** $K_{\text{gauss}}(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\sigma^2}\right)$, where $\|\mathbf{x} - \mathbf{x}'\|^2$ denotes the squared Euclidean distance between \mathbf{x} and \mathbf{x}' , and $\sigma > 0$ is a scale parameter controlling the width of the kernel. The Gaussian kernel is widely used due to its ability to model localized and highly non-linear interactions.

B Implementation details

B.1 Dataset description and process strategy

In this paper, we use datasets from the UCI repository for model validation, in alignment with the a recent NeurIPS-24 publication [1]. Detailed statistics for all selected datasets are provided in Tab. 4.

To simulate missing data, we first construct a binary mask matrix \mathbf{M} . The observed data matrix, denoted as $\mathbf{X}^{(\text{obs})}$, is derived by element-wise application of the complement mask $\mathbf{1} - \mathbf{M}$ to the fully observed data matrix $\mathbf{X}^{(\text{id})}$. Specifically, each entry $x_{nd}^{(\text{obs})}$ in $\mathbf{X}^{(\text{obs})}$ is given by $x_{nd}^{(\text{obs})} = x_{nd}^{(\text{id})}$ if $m_{nd} = 0$; otherwise, $x_{nd}^{(\text{obs})}$ is assigned the value Null. On the generation of \mathbf{M} , we consider three canonical missing data mechanisms:

- **Missing Completely at Random (MCAR):** The probability of entry-wise missingness is independent of both observed and unobserved data. To simulate MCAR, each entry of \mathbf{M} is independently set to 1 (missing) with probability p_{miss} , and to 0 (observed) with probability $1 - p_{\text{miss}}$.

Table 4: The statistics of involved datasets.

Abbreviation	Dataset Name	Number (N)	Dimension (D)
BT	Blood Transfusion	748	4
CC	Concrete Compression	1030	7
CBV	Connectionist Bench Vowel	990	10
IS	Ionosphere	351	34
PK	Parkinsons	195	23
QB	QSAR Biodegradation	1055	41
WQW	Wine Quality White	4898	11

Note. The column ‘Dimension’ and ‘Number’ denotes the number of variables and samples in each dataset, respectively.

- **Missing at Random (MAR):** The missingness of a variable depends only on values of observed variables [33, 32, 9]. To generate MAR scenarios, we randomly select a subset of features to be always observed. The missingness in the remaining features is simulated using a logistic regression model, where the observed features act as predictors. The model parameters are randomly initialized, and the intercept (bias) is calibrated to yield the desired missingness rate.
- **Missing Not at Random (MNAR):** The probability that a value is missing depends on the unobserved (missing) values themselves [34, 38, 11]. For MNAR simulation, we adopt the procedure in [1, 5]: the logistic model used for MAR is repurposed, but its inputs are themselves masked by an independent MCAR mechanism, making the missingness dependent on both observed and unobserved features.

B.2 Training protocols

To ensure reliable convergence, we set a maximum of 500 training iterations and adopt early stopping based on validation performance, using a patience parameter of 10 epochs. Optimization throughout is conducted using the Adam optimizer [6]. The kernel function is specified as the Gaussian kernel. The main hyperparameters, specifically the update rate η , batch size B, kernel number E and variance σ are determined by allocating 5% of the training data as a validation set and tuning over the intervals $\eta \in [0.0001, 0.01]$, $B \in [64, 512]$, $E \in [1, 7]$ and $\sigma \in [0.01, 10]$. All experiments are conducted on a hardware platform comprising two Intel(R) Xeon(R) Platinum 8383C CPUs (2.70GHz) and an NVIDIA GeForce RTX 4090 GPU.

On the implementation of baseline methods, we closely follow the implementation details in NewImp [1]. Hyperparameter reproducibility was confirmed in our environment, and we adopted the provided settings to run the baseline scripts and report the corresponding results of NewImp. The reproduction of other models also follows NewImp. Specifically, the batch size for ReMasker is set to 64, whereas for all other baseline models it is fixed at 512. The MIWAE model is configured with a latent dimension of 16 and 32 hidden units. The TDM model is implemented with two layers, each containing 16 hidden units. For the MIRACLE model, the number of hidden units is set to 32. ReMasker is implemented with an embedding dimension of 32, a depth of 6, a mask ratio of 0.5, encoder and decoder depths of 6 and 4 respectively, and uses 4 attention heads. Both MissDiff and CSDI-T are set with a channel size of 16, an embedding dimension of 128, and two layers. The diffusion step parameter is set to 100 for these models, and the number of particles is set to 50.

B.3 Evaluation metrics

The imputed data matrix $\mathbf{X}^{(\text{imp})}$ is evaluated to assess imputation quality. Following the protocol in [45], we primarily employ the modified mean absolute error (MAE) and root mean squared error (RMSE) for evaluation:

$$\text{MAE} := \frac{1}{\sum_{n=1}^N \sum_{d=1}^D \bar{m}_{nd}} \sum_{n=1}^N \sum_{d=1}^D \left| x_{nd}^{(\text{imp})} - x_{nd}^{(\text{obs})} \right| \bar{m}_{nd}, \quad (22)$$

$$\text{RMSE} := \sqrt{\frac{1}{\sum_{n=1}^N \sum_{d=1}^D \bar{m}_{nd}} \sum_{n=1}^N \sum_{d=1}^D \left\| x_{nd}^{(\text{imp})} - x_{nd}^{(\text{obs})} \right\|_2^2 \bar{m}_{nd}}, \quad (23)$$

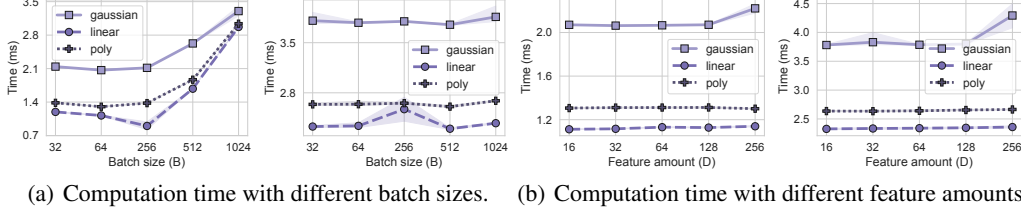


Figure 5: Running time of the forward pass (left panels) and backward pass (right panels) given varying settings. Different colors indicate different kernel functions. The colored lines and the shadowed areas indicate the mean values and the 99.9% confidence intervals.

where $\bar{m}_{nd} \in \bar{\mathbf{M}}$ indicates positions of imputed (originally missing) values with $\bar{m}_{nd} = 1 - m_{nd}$, and $x_{nd}^{(\text{obs})} \in \mathbf{X}^{(\text{obs})}$ is the ground-truth value from the fully observed data. As only the originally missing entries are imputed, we restrict the calculation of error metrics to the indices where $\bar{m}_{nd} = 1$.

In addition to the point-wise error metrics above, we also consider the squared Wasserstein distance (abbreviated as WASS) [1], which quantifies the discrepancy between the distributions of the imputed values and the corresponding ground-truth values at the missing positions ($\mathbf{M} = 1$).

C Additional experimental results

C.1 An empirical analysis on complexity

In this section, we examine the practical computational complexity of KPI. While the overall convergence was analyzed in Theorem ??, the computational cost per iteration, which includes both the forward and backward passes, has not been thoroughly discussed. To address this gap, we conducted experiments using Intel® Xeon® Gold 6140 CPUs and Nvidia RTX 4090 GPUs, with each experiment repeated 100 times to ensure reliability.

The results are presented in Fig. 5. **The running time per iteration remains limited (within 4 ms) across a diverse range of hyperparameters**, demonstrating the feasibility of KPI for real-world applications. Other key observations are summarized as follows:

- To explore the impact of batch size (B), we vary B within a wide range from 32 to 1024 while keeping the feature amount (D) to 8. The running cost of the forward pass increased with the batch size, as expected. This is attributed to the larger matrix inversion in (8), which cannot be efficiently accelerated by GPUs. In contrast, the backward pass cost was weakly correlated with B, since gradient computations after constructing the computation graph can be parallelized.
- To investigate the impact of feature amount (D), we maintain a constant batch size of 64. A weak correlation between D and the running time is observed. This is because varying D primarily affects the complexity of each kernel matrix computation, which can be effectively mitigated by GPU acceleration. This highlights a practical advantage of KPI: its efficiency in handling datasets with a large number of features.
- We observe that the type of kernel function also affects the running cost. The gaussian kernel exhibits the largest running time compared to other kernel functions, in terms of both forward pass and the backward pass.

C.2 Additional overall performance results given different missing ratios

Tab. 5-8 detail the imputation performance of KPI and baselines, with results for different missing ratios: 0.1, 0.2, 0.3, and 0.4 listed separately. The results demonstrate that KPI consistently outperforms the baselines in all settings, achieving superior performance in terms of both MAE and WASS. This consistent superiority across varying missing ratios underscores the effectiveness and robustness of KPI for missing data imputation.

Table 5: Imputation performance comparison with missing ratio of 0.1.

Datasets Metrics	BT		CC		CBV		IS		PK		QB		WQW	
	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS
MICE	0.118	0.027	0.155	0.075	0.196	0.16	0.175	0.406	0.097	0.133	0.122	0.271	0.192	0.151
Miss.F	0.123	0.037	0.172	0.111	0.185	0.149	0.141	0.295	0.128	0.163	0.102	0.284	0.164	0.129
Sinkhorn	0.840	0.434	0.903	0.614	0.896	0.837	0.850	2.047	0.841	1.513	0.784	2.622	0.856	0.755
TDM	0.724	0.415	0.815	0.545	0.787	0.690	0.720	1.592	0.731	1.295	0.565	1.977	0.745	0.650
CSDI-T	0.727	1.914	0.850	2.680	0.815	3.753	0.766	16.714	0.743	12.939	0.578	20.407	0.775	4.022
MissDiff	0.718	1.446	0.847	1.803	0.812	4.101	0.750	13.640	0.744	16.209	0.566	25.062	0.755	6.037
GAIN	0.739	0.355	0.759	0.479	0.690	0.541	0.532	1.137	0.399	0.460	0.409	1.192	0.736	0.621
MIRACLE	0.528	0.174	0.382	0.161	0.778	0.682	3.723	26.666	3.777	18.544	0.461	1.103	0.485	0.364
MIWAE	0.539	0.226	0.698	0.436	0.782	0.668	0.603	1.638	0.526	0.861	0.450	2.044	0.626	0.507
Remasker	0.365	0.099	1.041	0.830	0.448	0.249	0.715	1.775	0.500	0.739	0.489	1.737	0.503	0.364
NewImp	0.383	0.091	0.273	0.110	0.231	0.101	0.423	1.013	0.251	0.281	0.305	1.067	1.045	0.834
KPI(Ours)	0.084	0.022	0.023	0.01	0.051	0.016	0.093	0.217	0.071	0.066	0.05	0.219	0.082	0.058

Table 6: Imputation performance comparison with missing ratio of 0.2.

Datasets Metrics	BT		CC		CBV		IS		PK		QB		WQW	
	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS
MICE	0.145	0.027	0.171	0.097	0.208	0.218	0.186	0.915	0.102	0.243	0.13	0.589	0.2	0.211
Miss.F	0.141	0.058	0.173	0.131	0.187	0.206	0.144	0.589	0.133	0.316	0.106	0.579	0.168	0.181
Sinkhorn	0.834	0.428	0.907	0.711	0.902	1.079	0.842	3.908	0.819	2.572	0.773	5.036	0.854	1.030
TDM	0.725	0.431	0.812	0.659	0.800	0.939	0.720	3.097	0.710	2.167	0.567	3.855	0.750	0.927
CSDI-T	0.724	1.808	0.847	2.674	0.823	3.760	0.759	15.642	0.724	12.409	0.574	19.999	0.777	4.057
MissDiff	0.714	1.282	0.835	1.707	0.818	3.658	0.746	13.473	0.718	14.872	0.562	23.777	0.757	5.526
GAIN	0.727	0.350	0.759	0.585	0.701	0.739	0.526	2.231	0.409	0.830	0.407	2.292	0.724	0.853
MIRACLE	0.637	0.271	0.443	0.234	0.878	1.102	3.361	43.583	3.612	31.612	0.487	2.558	0.533	0.556
MIWAE	0.569	0.223	0.730	0.535	0.801	0.904	0.620	3.198	0.511	1.398	0.465	4.102	0.653	0.728
Remasker	0.403	0.108	0.412	1.223	0.488	0.392	0.613	2.959	0.450	1.077	0.397	2.482	0.523	0.531
NewImp	0.441	0.141	0.360	0.201	0.310	0.221	0.411	1.937	0.283	0.592	0.329	2.273	0.468	0.265
KPI(Ours)	0.095	0.032	0.077	0.051	0.085	0.064	0.098	0.436	0.075	0.128	0.062	0.322	0.103	0.11

Table 7: Imputation performance comparison with missing ratio of 0.3.

Datasets Metrics	BT		CC		CBV		IS		PK		QB		WQW	
	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS
mice	0.156	0.043	0.195	0.133	0.219	0.289	0.186	1.393	0.107	0.387	0.134	1.064	0.21	0.28
missforest	0.14	0.064	0.189	0.182	0.2	0.292	0.154	1.049	0.131	0.423	0.113	1.085	0.176	0.262
sink	0.828	0.475	0.911	0.853	0.904	1.368	0.851	6.014	0.828	3.898	0.774	7.291	0.859	1.313
tdm	0.733	0.506	0.825	0.834	0.809	1.260	0.730	4.796	0.723	3.337	0.571	5.629	0.754	1.240
CSDI-T	0.717	1.905	0.851	2.684	0.826	3.816	0.761	14.942	0.729	12.044	0.574	19.732	0.782	4.093
MissDiff	0.718	1.317	0.842	1.656	0.822	3.313	0.751	13.341	0.725	13.806	0.563	22.714	0.759	4.894
gain	0.742	0.413	0.780	0.729	0.736	1.041	0.566	3.702	0.460	1.656	0.434	3.637	0.730	1.140
miracle	0.951	0.850	0.535	0.371	0.841	1.302	3.036	54.592	3.432	43.764	0.542	4.814	0.582	0.792
miwae	0.593	0.273	0.769	0.692	0.818	1.210	0.650	4.974	0.527	2.113	0.480	5.810	0.667	0.955
remasker	0.459	0.134	0.552	0.371	0.541	0.586	0.534	3.949	0.415	1.365	0.349	2.928	0.557	0.724
NewImp	0.481	0.181	0.472	0.341	0.423	0.443	0.442	3.066	0.321	1.015	0.350	3.666	0.558	0.379
KPI(Ours)	0.104	0.028	0.116	0.088	0.122	0.122	0.102	0.712	0.083	0.217	0.069	0.562	0.148	0.215

Table 8: Imputation performance comparison with missing ratio of 0.4.

Datasets	BT		CC		CBV		IS		PK		QB		WQW	
	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS
MICE	0.162	0.03	0.223	0.168	0.233	0.354	0.186	1.824	0.111	0.549	0.15	1.491	0.222	0.329
MISS.F	0.156	0.083	0.198	0.226	0.192	0.346	0.154	1.346	0.133	0.595	0.114	1.254	0.177	0.326
Sinkhorn	0.837	0.530	0.904	1.008	0.889	1.616	0.847	7.810	0.821	4.948	0.768	9.508	0.860	1.582
TDM	0.737	0.596	0.824	1.037	0.802	1.561	0.733	6.376	0.724	4.367	0.578	7.565	0.758	1.574
CSDI-T	0.735	1.851	0.847	2.694	0.817	3.877	0.757	14.671	0.727	11.771	0.577	19.537	0.786	4.164
MissDiff	0.726	1.284	0.837	1.628	0.812	3.019	0.750	13.272	0.723	12.960	0.566	21.728	0.761	4.278
GAIN	0.712	0.464	0.812	0.960	0.791	1.448	0.665	6.203	0.522	2.708	0.653	11.553	0.826	1.767
Miracle	1.066	1.401	0.602	0.483	0.826	1.529	2.714	58.421	3.250	53.215	0.595	7.425	0.620	1.027
MIWAE	0.629	0.344	0.786	0.856	0.828	1.502	0.670	6.663	0.535	2.842	0.504	7.952	0.683	1.185
Remasker	0.528	0.182	1.022	1.541	0.636	0.860	0.534	5.653	0.424	1.891	0.368	4.096	0.601	0.926
NewImp	0.563	0.301	0.553	0.520	0.542	0.743	0.451	4.035	0.351	1.563	0.378	4.989	1.022	1.542
KPI(Ours)	0.113	0.039	0.132	0.134	0.144	0.191	0.107	1.022	0.09	0.337	0.084	1.028	0.159	0.303

C.3 Additional overall performance results given different missing mechanisms

Tab. 9 and 10 provide a detailed evaluation of the imputation performance of KPI and various baselines under MAR and MNAR mechanisms, respectively. These missing mechanisms are more complex and challenging compared to the MCAR setting reported in Tab. 1, but they are also more representative of real-world scenarios.

The results demonstrate that KPI consistently outperforms the baselines in all settings, achieving superior performance in terms of both metrics. This consistent superiority across different missing mechanisms highlights the effectiveness and robustness of KPI for missing data imputation, making it a reliable choice for diverse real-world applications.

C.4 Additional hyperparameter sensitivity results

Fig. 6 presents an extended analysis of hyperparameter sensitivity under higher missing ratios of 0.3 and 0.4, building upon the scenarios explored in Fig. 4 with missing ratios of 0.1 and 0.2. These additional experiments provide insights into the model’s behavior under more challenging conditions.

Overall, the model exhibits greater sensitivity to hyperparameter choices at higher missing ratios. This indicates that hyperparameter tuning becomes increasingly important as the missing ratio increases. However, despite the heightened sensitivity, the trends observed across different missing ratios remain consistent. For instance, the optimal update rate is found to be 0.01 for both CC and CBV across all four missing ratios. This consistency reduces the complexity of tuning the model for each specific missing ratio and implies that the selected hyperparameters for KPI are reliable and robust across a range of missing data scenarios.

Table 9: Imputation performance comparison under MAR missing mechanism.

Datasets	BT		CC		CBV		IS		PK		QB		WQW	
Metrics	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS
MICE	0.481	0.109	0.626	0.349	0.839	0.652	0.677	1.113	0.492	0.946	0.604	2.42	0.824	0.775
MISS.F	0.718	0.727	0.632	0.404	0.783	0.572	0.58	1.261	0.797	1.517	0.58	2.671	0.709	0.63
CSDI-T	1.094	5.465	0.894	3.212	0.826	4.286	0.707	15.194	1.262	19.116	0.782	23.176	0.815	4.919
MissDiff	1.019	2.835	0.888	2.189	0.852	6.008	0.704	13.233	1.219	22.773	0.762	34.125	0.805	6.919
gain	1.082	1.187	0.782	0.570	0.700	0.503	0.456	0.609	0.709	1.383	0.552	1.716	0.729	0.672
MIRACLE	0.699	0.510	0.356	0.141	0.710	0.530	3.837	19.874	4.518	23.842	0.605	1.636	0.494	0.385
MIWAE	0.747	0.784	0.735	0.517	0.788	0.617	0.474	0.811	0.758	1.674	0.660	2.892	0.629	0.575
Remasker	0.598	0.689	1.023	0.854	0.467	0.235	0.691	1.149	0.668	1.062	0.557	1.563	0.489	0.397
Sinkhorn	1.106	1.319	0.958	0.718	0.923	0.804	0.829	1.350	1.257	3.392	0.904	3.032	0.905	0.912
TDM	1.015	1.313	0.855	0.614	0.823	0.653	0.691	0.995	1.194	3.311	0.752	2.739	0.794	0.776
NewImp	0.401	0.171	0.232	0.111	0.221	0.070	0.331	0.504	0.462	0.745	0.560	3.330	0.372	0.293
multikip	0.367	0.107	0.199	0.121	0.225	0.115	0.345	0.864	0.457	0.68	0.339	1.965	0.362	0.311

Table 10: Imputation performance comparison under MNAR missing mechanism.

Datasets	BT		CC		CBV		IS		PK		QB		WQW	
Metrics	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS	MAE	WASS
MICE	0.696	0.411	0.66	0.384	0.832	0.734	0.708	1.831	0.499	0.98	0.589	2.377	0.807	0.724
MISS.F	0.731	0.579	0.697	0.483	0.748	0.631	0.587	1.944	0.726	1.513	0.5	2.291	0.667	0.567
CSDI-T	0.885	3.105	0.885	2.923	0.838	3.922	0.759	16.833	1.016	14.173	0.683	20.330	0.795	4.275
GAIN	0.846	0.595	0.782	0.545	0.698	0.570	0.529	1.151	0.571	1.305	0.474	1.943	0.730	0.684
MIRACLE	0.655	0.319	0.371	0.163	0.842	0.802	3.725	27.093	4.196	25.052	0.576	2.249	0.518	0.437
MIWAE	0.658	0.424	0.735	0.508	0.808	0.731	0.559	1.535	0.628	1.400	0.561	3.318	0.641	0.577
Remasker	0.481	0.297	1.028	0.886	0.487	0.296	0.660	1.701	0.586	1.059	0.516	2.128	0.519	0.434
Sinkhorn	0.967	0.752	0.940	0.698	0.925	0.911	0.854	2.121	1.049	2.906	0.844	3.755	0.880	0.859
TDM	0.858	0.732	0.849	0.620	0.821	0.756	0.724	1.640	0.969	2.713	0.661	3.202	0.772	0.744
NewImp	0.645	0.461	0.585	0.593	0.562	0.837	0.442	3.945	0.434	2.328	0.441	7.161	0.601	1.102
multikip	0.573	0.257	0.271	0.22	0.357	0.352	0.391	1.344	0.423	0.769	0.286	1.967	0.458	0.563

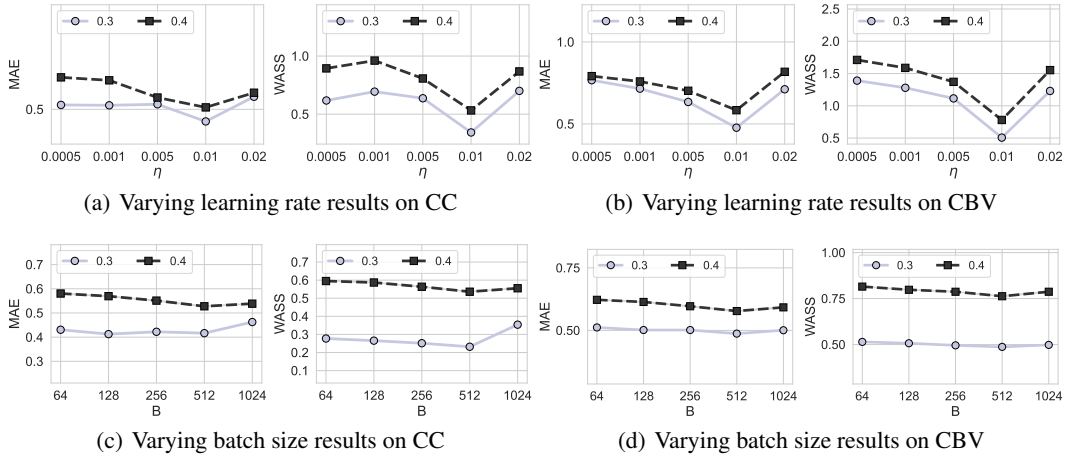


Figure 6: Varying learning rate and batch size results with missing ratios 0.3 and 0.4.

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