Beyond Impute-Then-Regress: Adapting Prediction to Missing Data

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Missing values are a common issue in real-world datasets. The gold standard for dealing with missing data in inference is to assume that the data is missing at random and apply an impute-then-estimate procedure. In this paper, we evaluate the relevance of the assumptions and methods developed in inference for prediction tasks. We first provide a theoretical analysis of impute-then-regress methods and highlight their successes and failures in making accurate predictions. We propose adaptive linear regression, a new class of models that adapt to the set of available features and can be applied on partially observed data directly. We show that adaptive linear regression can be equivalent to impute-then-regress methods where the imputation and the linear regression models are learned simultaneously instead of sequentially. We leverage this joint-impute-then-regress interpretation to generalize our framework to non-linear models. We validate our theoretical findings and adaptive regression approaches with extensive numerical results on synthetic, semi-synthetic, and real-world datasets. Among others, in settings where data is strongly not missing at random, our methods achieve a 6% improvement in out-of-sample accuracy.

Key words: Missing data; Imputation; Linear regression; Adaptive optimization.

1. Introduction

Real-world datasets usually combine information from multiple sources, with different measurement units, data encoding, or structure, leading to a myriad of inconsistencies. In particular, they often come with some partially observed features. In contrast, most supervised learning models require that a fixed set of input features is available for every data

point. Though helpful to develop new methods, this assumption has become increasingly divorced from the modern data reality.

The problem of missing data is not new in statistics and has been a topic of study for several decades (see, for instance, Little and Rubin 2019). For inference purposes, the key assumption is that data entries are missing at random (MAR) – i.e., the fact that a feature is missing and its (unobserved) value are independent, conditional on the observed features. Under the MAR assumption, a valid inference methodology, for example, is to impute-then-estimate, i.e., impute the missing values as accurately as possible, estimate the parameter of interest on the imputed dataset, and obtain valid confidence intervals by accounting for potential imputation errors (e.g., via multiple imputations as in Rubin 1987). However, most inference guarantees become invalid as soon as the data is not missing at random (NMAR), and, without any further assumptions about the data, the MAR assumption cannot be tested nor refuted from the data (see Little 1988, Jaeger 2006, for some additional assumptions amenable to statistical testing).

However, prediction is a different task from inference (Shmueli et al. 2010) and, as we argue in this paper, requires a different treatment for missing data. The current state-of-practice for prediction with missing data mimics the gold standard for inference, namely uses an *impute-then-regress* approach in which one first imputes missing values, and then trains a model on the imputed dataset. Accordingly, the MAR assumption, which is required for the imputation step to be unbiased, is often perceived as a requirement for impute-then-regress approaches. For prediction, however, MAR is not required. Indeed, we will show that some impute-then-regress methods can be 'optimal' even when the data is NMAR and we also establish conditions in Section 3.4 under which the predictive accuracy benefits from data NMAR.

Such observations motivate this paper's goal to re-evaluate the state of practice for prediction tasks in the presence of missing data.

Contributions. We begin from the current state of practice, namely impute-then-regress, and study the consistency of generic imputation rules in the infinite-data regime. Our result generalizes the analysis of mean-impute-then-regress under MAR of Josse et al. (2019) to cases with discrete features, generic imputation rules, and where MAR is not satisfied. Surprisingly, we find that inference and prediction endorse completely different imputation methods. Inference requires the imputed values to be unbiased estimates of the missing

entries (a property usually satisfied under MAR), and with as small imputation error as possible. On the contrary, for prediction, impute-then-regress works if the imputed value codifies missingness, i.e., if the imputed values are as conspicuous as possible. However, this analysis holds in the limit of infinite data.

For increased predictive accuracy with finite data, we propose two alternative approaches for handling missing data in practice. We first develop a novel linear regression framework in which the predictive model adapts to the set of available features. More precisely, we treat prediction with missing data as a two-stage problem in which we first observe which features are missing, then choose a predictive model to apply to the observed features. The two-stage view allows us to propose a hierarchy of adaptive models following the principles of adaptive robust optimization. In some special cases, we show that adaptive linear models are equivalent to impute-then-regress where the imputation and prediction models are learned jointly instead of sequentially. Based on this insight, we propose a second approach, which naturally extends adaptive linear regression to non-linear models, in which we jointly train a simple imputation model (for missing features) and an arbitrary non-linear prediction model (for the target variable) using alternating optimization.

We extensively benchmark impute-then-regress strategies and our algorithms on numerical experiments with synthetic, semi-synthetic (i.e., real-world design matrix and missingness patterns but synthetic signals), and real-world data. We find that all methods perform comparably when data is missing at random but that our two proposals outperform state-of-practice quite significantly when data is not missing at random. Since the MAR assumption cannot be tested from the data itself, the true missingness mechanism is always unknown in practice and models that enjoy robust performance irrespective of the missingness mechanism are highly desirable.

Outline. Section 2 reviews the literature on missing data mechanisms and imputation methods, and highlights key differences between inference and prediction settings, in particular revisiting the relevance of missing data mechanisms proposed with inference in mind. We then consider impute-then-regress methods and analyze the theoretical (in)consistency of simple missing data imputation rules in Section 3. We discuss the consistency of mode and mean imputation, and confirm these theoretical findings empirically on semi-synthetic and real data. In Section 4 we propose the adaptive linear regression framework and provide finite-sample generalization bounds for our hierarchy of models. We connect adaptive

linear regression to optimal joint-impute-then-regress in Section 5. Based on this connection, we propose a heuristic joint impute-then-regress learning algorithm for non-linear models, which we validate on synthetic data. Finally, in Section 6, we compare the performance of the the state-of-practice impute-then-regress strategies analyzed in Section 3 with that of adaptive linear regression (Section 4) and joint impute-then-regress (Section 5) on semi-synthetic and real-world instances.

Notation. We denote scalars by lowercase characters (x) and random variables by uppercase characters (X). Boldfaced characters denote vectors (e.g. x is a vector and X is a random vector). The symbol \bot designates independent random variables. For any positive integer n, let $[n] = \{1, \ldots, n\}$. We typically consider n i.i.d. samples (x_i, m_i) , $i \in [n]$, where $x_i \in \mathbb{R}^d$ is the vector of covariates and $m_i \in \{0, 1\}^d$ is a vector indicating the missing covariates, i.e., $m_{ij} = 1$ if x_{ij} is missing, 0, otherwise. For every data point i, $||m_i||_0 := \sum_j m_{ij}$ covariates are missing. We refer to m_i as the missingness indicator or missingness pattern of sample i. We further denote $o(x_i, m_i)$ the $(d - ||m_i||_0)$ -dimensional vector of observed covariates (Seaman et al. 2013). Symmetrically, $o(x_i, 1 - m_i)$ is the vector of unobserved ones. With these notations, $(x_i, m_i)_{i \in [n]}$ corresponds to the dataset of realizations while $(o(x_i, m_i), m_i)_{i \in [n]}$ is the dataset of observations.

2. Related work

In this section, we review the literature on missingness mechanisms and methods for inference with missing data.

2.1. Missingness mechanisms

Missingness mechanisms model why the data is missing and inform how to design analysis strategies. In the context of parameter estimation via likelihood maximization, Rubin (1976) introduced three missing data mechanisms, which we state below. Because these classical definitions were introduced with inference in mind, they do not distinguish the dependent or target variable Y from the input vector X.

Assume that the realized dataset is sampled i.i.d. from a distribution in $\mathcal{F} = \{g(\boldsymbol{x};\boldsymbol{\theta})h(\boldsymbol{m}|\boldsymbol{x};\boldsymbol{\phi}): (\boldsymbol{\theta},\boldsymbol{\phi})\in\Omega\}$, where $\boldsymbol{\theta}$ parametrizes the density of the fully observed data, $g(\cdot;\boldsymbol{\theta})$, while $\boldsymbol{\phi}$ parametrizes the density function of the missingness pattern \boldsymbol{m}

conditioned on x, denoted by $h(\cdot|x;\phi)$. The likelihood of the observed data is given by integrating over the missing values

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}) = \prod_{i=1}^{n} \int g(\boldsymbol{x}; \boldsymbol{\theta}) h(\boldsymbol{m}_{i} | \boldsymbol{x}; \boldsymbol{\phi}) \delta_{\boldsymbol{o}(\cdot, \boldsymbol{m}_{i}) = \boldsymbol{o}(\boldsymbol{x}_{i}, \boldsymbol{m}_{i})}(\boldsymbol{x}) d\boldsymbol{x}, \tag{1}$$

where δ is the standard Dirac measure. The parameter $\boldsymbol{\theta}$, which controls the data generating process, is often more of interest than the missingness generating process and $\boldsymbol{\phi}$. However, in general, the two parameters need to be estimated jointly. Rubin (1976) noted that joint estimation is much easier under a mechanism called Missing At Random:

DEFINITION 1. Missing data are called *missing at random* (MAR) if, conditioned on the observed covariates o(X, M), the missingness indicator M is independent of the unobserved covariates o(X, 1-M).

Under MAR, the term $h(\boldsymbol{m}_i|\boldsymbol{x};\boldsymbol{\phi})$ in (1) only depends on $\boldsymbol{o}(\boldsymbol{x},\boldsymbol{m}_i) = \boldsymbol{o}(\boldsymbol{x}_i,\boldsymbol{m}_i)$. Hence, $\boldsymbol{\theta}$ can be estimated independently of $\boldsymbol{\phi}$ by maximizing the partial likelihood, i.e., (1) without the $h(\boldsymbol{m}_i|\boldsymbol{x};\boldsymbol{\phi})$ term. A stronger assumption than MAR is Missing Completely At Random (MCAR), under which \boldsymbol{M} is assumed independent of the covariates \boldsymbol{X} . Under MCAR, the marginal density function $g(\boldsymbol{m}|\boldsymbol{x};\boldsymbol{\phi})$ does not depend on \boldsymbol{x} . Finally, we say that the missing data is *Not Missing At Random* (NMAR) if MAR is not satisfied.

We emphasize two limitations of the above definitions in a predictive setting. First, these definitions apply to a single dataset with no distinction between training and test sets, which is a common distinction in supervised learning tasks. Second, the target response Y is not explicitly considered when defining the missingness mechanisms. At best, we can consider Y as part of the input X. However, Y is a unique variable –for example, it cannot be missing– and we argue it deserves specific treatment.

2.2. Inference with missing data and multiple imputation

Techniques to deal with missing data in inference settings can be divided into two independent directions, expectation-maximization (EM) approaches and imputation. For maximum likelihood estimation tasks, such as the one presented in Section 2.1, Dempster et al. (1977) proposed a variant of the EM algorithm which provides unbiased estimators even in presence of missing data, under the MAR assumption. To derive confidence intervals, one can then estimate the variance of these estimates using the supplemented EM algorithm (Meng and Rubin 1991) or Louis' formula (Louis 1982). However, implementation of these

techniques are not straightforward and dedicated algorithms must be designed even for the most common estimation tasks, such as generalized linear models (Ibrahim et al. 2005) or logistic regression (Jiang et al. 2020).

Alternatively, one can implement an impute-then-estimate strategy. An imputation method is a procedure that takes as input a dataset of observations $(o(x_i, m_i), m_i)_{i \in [n]}$ and returns an imputed dataset $(\tilde{x}_i)_{i \in [n]}$, where $\tilde{x}_i \in \mathbb{R}^d$. A myriad of imputation techniques have been proposed based on mean and mode imputation (Little and Rubin 2019), k-nearest neighbors (Troyanskaya et al. 2001, Brás and Menezes 2007), least square regression (Bø et al. 2004, Kim et al. 2005, Cai et al. 2006, Zhang et al. 2008), support vector machine/regression (Wang et al. 2006, Bertsimas et al. 2018), decision trees (Bertsimas et al. 2018), neural networks (Yoon et al. 2018), or factor analysis and other dimension reduction techniques (Mohamed et al. 2009, Husson et al. 2019). In an ideal world, a perfect imputation method would return the best estimate of the full data given the observed information, namely

$$\tilde{oldsymbol{x}}_i = \mathbb{E}\left[oldsymbol{X}_i \ \middle| \left\{oldsymbol{o}(oldsymbol{X}_{i'}, oldsymbol{m}_{i'}) = oldsymbol{o}(oldsymbol{x}_{i'}, oldsymbol{m}_{i'})
ight\}_{i' \in [n]}
ight].$$

Then, one can estimate the parameter of interest on the imputed data $(\tilde{x}_i)_{i \in [n]}$.

For example, assume that we have access to a valid estimation procedure for some parameter θ (e.g., a particular coefficient in a linear regression model), i.e., a function that maps a dataset of full observations $\{x_i\}_{i\in[n]}$ to an estimate for θ , $\hat{\theta}\left(\{x_i\}_{i\in[n]}\right)$. Typically, the estimator should be unbiased, i.e., $\mathbb{E}\left[\hat{\theta}\left(\{X_i\}_{i\in[n]}\right)\right] = \theta$. The objective in a missing data setting is to compute

$$\mathbb{E}\left[\hat{\theta}\left(\left\{\boldsymbol{X}_{i}\right\}_{i\in[n]}\right)\middle|\left\{\boldsymbol{o}(\boldsymbol{X}_{i'},\boldsymbol{m}_{i'})=\boldsymbol{o}(\boldsymbol{x}_{i'},\boldsymbol{m}_{i'})\right\}_{i'\in[n]}\right],\tag{2}$$

which is not the same as the result from naive impute-then-estimate, $\hat{\theta}\left(\{\tilde{x}_i\}_{i\in[n]}\right)$. In particular, for the ideal imputation method mentioned above, impute-then-estimate yields

$$\hat{ heta}\left(\left\{ ilde{oldsymbol{x}}_{i}
ight\}_{i\in[n]}
ight)=\hat{ heta}\left(\left\{\mathbb{E}\left[X_{i}\,|\left\{oldsymbol{o}(oldsymbol{X}_{i'},oldsymbol{m}_{i'})=oldsymbol{o}(oldsymbol{x}_{i'},oldsymbol{m}_{i'})
ight\}_{i'\in[n]}
ight)$$

which is not equivalent to (2) due to the inverted order of the estimation step $\hat{\theta}(\cdot)$ and the expectation step.

To avoid the pitfalls of single imputation, Rubin (1987) proposed the use of multiple imputed datasets. A multiple imputation method returns not one but a collection of imputed

datasets $(\tilde{x}_i^{(j)}, i \in [n])$ for $j \in [k]$, which can be interpreted as k independent samples from the distribution of

$$\{m{X}_i\}_{i\in[n]} \mid \{m{o}(m{X}_{i'},m{m}_{i'}) = m{o}(m{x}_{i'},m{m}_{i'})\}_{i'\in[n]}$$

By estimating θ on each imputed dataset individually and combining the results using Rubin's rule, we indeed recover unbiased estimates of the parameter θ and its variance under the MAR assumption. In practice, multiple imputation can be performed using sequential regression (Raghunathan et al. 2001), sequential decision trees (Burgette and Reiter 2010) or random forests (Stekhoven and Bühlmann 2012).

2.3. Contrasting the inference and prediction settings

In supervised learning, the goal is to predict a response Y based on the vector of covariates X. The prediction task can be reduced to an inference setting, by considering predictions of the form $f(x; \theta)$, where $\theta \in \Omega$ and $\{f(\cdot, \theta) : \theta \in \Omega\}$ is a fixed class of learners, and solving an empirical risk minimization problem of the form

$$\hat{\boldsymbol{\theta}} \in \arg\min_{\boldsymbol{\theta} \in \Omega} \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(\boldsymbol{x}_i; \boldsymbol{\theta})),$$

where the loss function $\ell(\cdot,\cdot)$ measures the prediction error. The loss function is chosen to produce asymptotically consistent predictors:

DEFINITION 2. A predictor \hat{f}_n trained on a complete (i.e., no missing entries) dataset of n observations is (asymptotically) consistent if $\lim_{n\to\infty} \hat{f}_n(\mathbf{x}) = \mathbb{E}[Y|\mathbf{X}=\mathbf{x}]$. Moreover, \hat{f}_n is universally consistent if the previous statement holds for any distribution of (\mathbf{X}, Y) .

Despite significant focus on predictive modeling in recent years, the state of practice for dealing with missing data remains firmly inspired by the insights drawn from inference and typically consists of three alternatives. For example, Hastie et al. (2001, chapter 9.3) recommends:

"Assuming the features are missing completely at random, there are a number of ways of proceeding:

(1) Discard observations with any missing values. (2) Rely on the learning algorithm to deal with missing values in its training phase. (3) Impute all missing values before training. [...] For most learning methods, the imputation approach (3) is necessary."

First, MAR (here, MCAR) is presented as a fundamental requirement, a clear heritage from the inference literature. Among the three options proposed, both options (1) and (3) are direct adaptations of techniques developed for inference.

Option (1), a.k.a. complete-case analysis, might be applicable when calibrating the model f but is not satisfactory when a predictive model deployed in real-life encounters input with missing entries.

Option (2) refers to specific model classes that can naturally deal with input with missing entries. Since the vector o(x, m) does not have a fixed dimension, one can instead consider the extended vector $e(x, m) \in (\mathbb{R} \cup \{\text{NA}\})^d$ where the missing entries are encoded via a specific value NA, and consider functions f that can account for the half-discrete nature of its argument e(x, m). To the best of our knowledge, only tree-based methods are currently able to cope with such features. The Missingness Incorporated as Attribute (MIA) technique (Twala et al. 2008) constructs splits that apply directly on the extended vector and is the state-of-the-art for treating missing values in decision trees (see Josse et al. 2019, section 6, for a numerical comparison).

Option (3) corresponds to the standard impute-then-estimate strategy applied to the empirical risk minimization problem above, viewed as an inference task. As we discussed in Section 2.2, a simple impute-then-predict approach (though widely common in practice) would incur bias in parameter estimation. Alternatively, one should perform multiple imputations of the training set and compute a family of models $f(\cdot, \hat{\boldsymbol{\theta}}^{(1)}), \dots, f(\cdot, \hat{\boldsymbol{\theta}}^{(k)})$. Having multiple models, however, might lead to issues related to storage, tractability, and interpretability. As a result, multiple imputation methods are often eschewed in practice, in favor of less theoretically sound single imputation methods.

Kuhn et al. (2013, chapter 3.4) makes identical recommendations as Hastie et al. (2001)¹ and imputation is the approach receiving the most detailed treatment in both textbooks, as well as in Gelman and Hill (2006). Imputation techniques and the missing at random (MAR) assumption they require have been so successful in inference that their relevance in prediction is rarely questioned.

However, prediction has two salient characteristics that are absent from inference. First, the goal in prediction is to guess as accurately as possible the output Y. The accuracy (or even the bias) in the estimation of the parameters of the predictive model, θ , is secondary. Second, predictive models are intended to be deployed in software/IT tools and applied to new observations on the fly. Accordingly, any processing of the data required

¹ "If we do not remove the missing data, there are two general approaches. First, a few predictive models, especially tree-based techniques, can specifically account for missing data. [...] Alternatively, missing data can be imputed."

to calibrate f must be applicable out-of-sample, to new observations. For example, for impute-then-regress, if a new observation has missing entries, they have to be imputed before applying f. The literature from inference suggests that applying the predictor rule f to a single imputed version of the observation may lead to biased prediction, but performing multiple imputations and averaging predictions, although unbiased, requires additional computational time and storage resources (Josse et al. 2019, section 4.1). This violates the assumption that computing predictions from a previously trained model is fast, computationally efficient, and can be performed in an online and/or embedded fashion—an assumption which is critical for many applications of machine learning.

In short, though multiple imputation is the "gold standard" for statistical inference with missing data, applying it in a prediction setting can be computationally challenging. If data are missing in both the training and testing set, it may be necessary to train multiple models, then evaluate each one on multiple imputed versions of each out-of-sample data point. It is therefore of interest to study the impact of missing data on the predictive task directly and investigate methods that do not require any sophisticated imputation.

3. Evaluation of simple impute-then-regress strategies

In practice, impute-then-regress strategies are prevalent due to their ease of implementation. Hence, understanding how and whether they negatively impact the learned prediction rule are crucial questions to answer. In this section, we theoretically and empirically explore the quality of simple rules like mean or mode-imputation for prediction. As Josse et al. (2019), we consider a simplified setting in d dimensions where only the first covariate X_1 is missing, but the analysis could be generalized to multiple missing features (see Josse et al. 2019, section 4.2). In this setting, the optimal (consistent) predictor is predicting

$$\begin{cases}
\mathbb{E}[Y|\mathbf{X} = \mathbf{x}, M_1 = 0], & \text{if } m_1 = 0, \\
\mathbb{E}[Y|\mathbf{X}_{2:d} = \mathbf{x}_{2:d}, M_1 = 1], & \text{if } m_1 = 1.
\end{cases}$$
(3)

Here, we concisely denote $x_{2:d}$ the (d-1)-dimensional vector (x_2, \ldots, x_d) . In Section 3.1, we derive generic necessary and sufficient conditions for the consistency of generic impute-then-regress strategies, which generalize the analysis of mean impute-then-regress of Josse et al. (2019, section 4.2). We then discuss the theoretical implications for mode (resp. mean) imputation and verify empirically these findings in Section 3.2 (resp. Section 3.3).

3.1. Consistency of generic imputation rules

We study the common practice of imputing a deterministic value $\mu(\mathbf{x}_{2:d})$ on the training set and its impact on the downstream prediction task. This model captures mean and mode imputation, conditional mean and mode imputation, and more generally any method that deterministically imputes a value for X_1 as a function of the other covariates $\mathbf{x}_{2:d}$, $\mu(\mathbf{x}_{2:d})$. For clarity, we will denote \mathbf{X}^{μ} the random variable obtained from (\mathbf{X}, \mathbf{M}) after μ -imputation, i.e., $X_1^{\mu} = X_1$ if $M_1 = 0$, $\mu(\mathbf{X}_{2:d})$ otherwise.

THEOREM 1. Consider a universally consistent learning algorithm when trained on any fully observed dataset. Systematically imputing $\mu(\mathbf{x}_{2:d})$ for $X_1|\mathbf{X}_{2:d}=\mathbf{x}_{2:d}$ on the training set and training a predictor on the imputed dataset leads, in the limit with infinite data, to the following prediction rule, denoted $f_{\mu-impute}(\mathbf{x})$ and equal almost everywhere to

$$\begin{cases} \mathbb{E}[Y|\boldsymbol{X} = \boldsymbol{x}, M_1 = 0], & \text{if } x_1 \neq \mu(\boldsymbol{x}_{2:d}), \\ \alpha(\boldsymbol{x})\mathbb{E}[Y|\boldsymbol{X}_{2:d} = \boldsymbol{x}_{2:d}, M_1 = 1] + (1 - \alpha(\boldsymbol{x}))\mathbb{E}[Y|X_1 = \mu(\boldsymbol{x}_{2:d}), \boldsymbol{X}_{2:d} = \boldsymbol{x}_{2:d}, M_1 = 0], & \text{o.w.,} \end{cases}$$

where

- $\eta(\boldsymbol{x}) = \mathbb{P}(M_1 = 1 | \boldsymbol{X}_{2:d} = \boldsymbol{x}_{2:d})$ is the probability that X_1 is missing given $\boldsymbol{X}_{2:d}$,
- $p_{\mu}(\boldsymbol{x}) = \mathbb{P}(X_1 = \mu(\boldsymbol{x}_{2:d}), M_1 = 0 | \boldsymbol{X}_{2:d} = \boldsymbol{x}_{2:d})$ is the probability for the true X_1 to take the imputed value $\mu(\boldsymbol{x}_{2:d})$ and not be missing, given the other covariates,
- and $\alpha(\mathbf{x}) = \frac{\eta(\mathbf{x})}{\eta(\mathbf{x}) + p_{\mu}(\mathbf{x})}$ is the posterior probability that X_1 was missing before imputation, given that it takes the value $\mu(\mathbf{x}_{2:d})$ after imputation, i.e., $\mathbb{P}(M_1 = 1 | X_1^{\mu} = \mu(\mathbf{x}_{2:d}), \mathbf{X}_{2:d} = \mathbf{x}_{2:d})$.

We defer the proof to Appendix A. Intuitively, in the infinite-data regime, only the training data in the neighborhood of \boldsymbol{x} affect the prediction. In the first case, \boldsymbol{x} is locally surrounded by points with no missing entries (almost surely). In the second case, however, the points in the neighborhood of \boldsymbol{x} come from a mixture of two distributions: either $(\mu(\boldsymbol{x}_{2:d}), \boldsymbol{X}_{2:d})|M_1 = 1$ in the case where X_1 is missing, or $(X_1, \boldsymbol{X}_{2:d})|M_1 = 0$. So, the predicted outcome is a weighted average of both conditional expectations, with $\alpha(\boldsymbol{x})$ being the proper weighting factor.

REMARK 1. Observe that $\alpha(\boldsymbol{x}) \neq \eta(\boldsymbol{x}) = \mathbb{P}(M_1 = 1 | \boldsymbol{X}_{2:d} = \boldsymbol{x}_{2:d})$ in general. Even when X_1 and M_1 are conditionally independent (i.e., MAR assumption), imputation induces correlation between X_1^{μ} and M_1 .

We now apply Theorem 1, to study the out-of-sample predictions from a learner trained on μ -imputed data. For a new observation $(\boldsymbol{o}(\boldsymbol{x}, m_1), m_1)$, we apply μ -imputation if needed and then predict according to $f_{\mu-impute}(\boldsymbol{x})$. If $m_1 = 0$, the impute-then-predict rule yields

$$\begin{cases} \mathbb{E}[Y|\boldsymbol{X} = \boldsymbol{x}, M_1 = 0], & \text{if } x_1 \neq \mu(\boldsymbol{x}_{2:d}), \\ \alpha(\boldsymbol{x})\mathbb{E}[Y|\boldsymbol{X}_{2:d} = \boldsymbol{x}_{2:d}, M_1 = 1] + (1 - \alpha(\boldsymbol{x}))\mathbb{E}[Y|X_1 = \mu(\boldsymbol{x}_{2:d}), \boldsymbol{X}_{2:d} = \boldsymbol{x}_{2:d}, M_1 = 0], & o.w. \end{cases}$$

For this rule to agree with the Bayes-optimal predictor, $\mathbb{E}[Y|\mathbf{X}=\mathbf{x},M_1=0]$, almost everywhere, we need either the second case to happen with probability zero or $\alpha(\mathbf{x})=0$. If X_1 is continuous, for example, then $\mathbb{P}(X_1=\mu(\mathbf{x}_{2:d}))=0$ so the former condition is satisfied by design. If X_1 is discrete, choosing $\mu(\mathbf{x}_{2:d})$ outside of the original support of X_1 , i.e., $\mathbb{P}(X_1=\mu(\mathbf{x}_{2:d}))=0$, provides consistency.

If $m_1 = 1$, then x_1 is replaced by its imputed value $\mu(\boldsymbol{x}_{2:d})$ so the impute-then-predict rule yields

$$\alpha(\boldsymbol{x})\mathbb{E}[Y|\boldsymbol{X}_{2:d} = \boldsymbol{x}_{2:d}, M_1 = 1] + (1 - \alpha(\boldsymbol{x}))\mathbb{E}[Y|X_1 = \mu, \boldsymbol{X}_{2:d} = \boldsymbol{x}_{2:d}, M_1 = 0],$$

which agrees with the Bayes-optimal estimator $\mathbb{E}[Y|X_{2:d}=\boldsymbol{x}_{2:d},M_1=1]$ iff $\alpha(\boldsymbol{x})=1$. Again, $\alpha(\boldsymbol{x})$ corresponds to the posterior probability that X_1 was missing in the original observation given that $X_1^{\mu}=\mu(\boldsymbol{x}_{2:d})$. In other words, Theorem 1 indicates that consistency is achieved as long as the predictor can almost surely de-impute, that is properly guess after imputation whether X_1 was originally missing or not. This discussion can be summarized by the following corollary:

COROLLARY 1. Under the assumptions and notations of Theorem 1, μ -imputation-thenregress asymptotically (i.e., in the infinite-data regime) leads to Bayes-optimal estimates at \boldsymbol{x} if and only if $\alpha(\boldsymbol{x}) = 1$.

Consequently, despite the simplicity of the underlying intuition, Theorem 1 challenges common practice. Indeed, one could think that a good imputation method should produce datasets that are plausible, i.e., where imputed and non-imputed observations are undistinguishable ($\alpha(\mathbf{x}) = 0$). On the contrary, as far as predictive power is concerned, Theorem 1 speaks in favor of imputation methods that can be surely de-imputed ($\alpha(\mathbf{x}) = 1$), because they can be used as an encoding for missingness.

3.2. Categorical/discrete variables: Mode imputation is inconsistent

For discrete features, choosing μ as the mode of the distribution of $X_1|M_1=0$ (a.k.a. mode imputation) is one of the advised methods in practice. However, with this choice of μ , $p_{\mu}(\boldsymbol{x}) > 0$ so $\alpha(\boldsymbol{x}) < 1$ and mode impute-then-regress cannot be asymptotically consistent by Corollary 1. Conversely, choosing μ outside of the original support of X_1 , i.e., encoding missingness as a new category/value, provides consistency.

The practical implications of Corollary 1 for categorical variables are thus clear: We should encode missingness as a new category instead of imputing the mode. Accordingly, we numerically compare the out-of-sample performance of these two approaches.

Our analysis comprises the 41 datasets with at least one missing categorical feature described in Tables 5 and 7 in Appendix E.2. We consider both synthetic (linear and neural network) and real signals Y (available for 35 out of the 41 datasets). For synthetic signals, the missingness pattern can be missing at random (MAR), not missing at random (NMAR) or adversially missing (AM) as described in Appendix E.2. For training predictive models, missing numerical features are mean-imputed and missing categorical are either encoded as their own category or mode-imputed. The downstream predictive model is chosen among a regularized linear, tree, and a random forest model (using 5-fold cross-validation on the training data).

To quantitatively assess the effect of mode imputation, we compare the out-of-sample accuracy with and without mode imputation using a paired t-test (difference in means) and paired Wilcoxon test (difference in pseudo-medians). Results are reported in Table 1. We observe that mode imputation has a clear significant negative (detrimental) effect on predictive power on instances with synthetic signals, hence corroborating the insights from Theorem 1. Yet, we do not observe a significant effect when we predict the real signal Y, which suggests that other factors beyond missing data might impact the validity of Theorem 1 in practice (e.g., finite amount of samples, limited class of predictors).

3.3. Continuous variables: Mean imputation is consistent

For continuous features, one of simplest and most widely used imputation rule is mean imputation, namely using $\mu = \mathbb{E}[X_1|M_1=0]$. Further assume that $X_1|\mathbf{X}_{2:d} = \mathbf{x}_{2:d}, M_1=0$ is continuous (i.e., if the 'observed' X_1 is continuous, conditioned on the other covariates), then, conditioned on $\mathbf{X}_{2:d} = \mathbf{x}_{2:d}$ and $M_1 = 0$, the probability that X_1 takes any specific value is 0 so $p_{\mu}(\mathbf{x}) = 0$ and $\alpha(\mathbf{x}) = 1$. Consequently, Corollary 1 guarantees that mean

Table 1 Difference in means and in pseudo-medians (with one-sided *p*-values) in out-of-sample accuracy from a *t* and Wilcoxon test applied to assess the impact of mode imputation on downstream accuracy. A negative impact means that mode imputation reduces accuracy.

Signal Y	Missingness	Δ mean (p-value)	Δ pseudo-median (p-value)
	MAR	$-0.0569 \ (< 10^{-22})$	$-0.0303 \ (< 10^{-22})$
Synthetic - Linear	NMAR	$-0.0396 \ (< 10^{-22})$	$-0.0098 \ (< 10^{-22})$
	AM	$-0.0527 \ (< 10^{-22})$	$-0.0235 \ (< 10^{-22})$
	MAR	$-0.0271 \ (< 10^{-22})$	$-0.0063 \ (< 10^{-22})$
Synthetic - NN	NMAR	$-0.0317 \ (< 10^{-22})$	$-0.0053 \ (< 10^{-22})$
	AM	$-0.0284 \ (< 10^{-22})$	$-0.0059 \ (< 10^{-22})$
Real	Real	0.0044 (0.77)	-0.001 (0.19)

imputation-then-regress is asymptotically consistent, as already proved by Josse et al. (2019, theorem 4). Intuitively, systematically imputing μ for X_1 creates a discontinuity in the distribution of X_1^{μ} and the events $\{X_1^{\mu} = \mu\}$ and $\{M_1 = 1\}$ are equal almost surely. The downstream predictive model (since it is universally consistent) is then able to learn this pattern and view $X_1^{\mu} = \mu$ as an encoding for missingness.

In practice, this result suggests that sophisticated imputation methods for continuous variables are not needed, and may indeed be counter-productive. We now empirically evaluate the validity of this finding.

We consider the 52 datasets with at least one missing numerical feature described in Tables 7 and 6 in Appendix E.2. As for mode imputation in the previous section, We consider both real signals Y (available for 37 out of the 52 datasets) and synthetic ones (linear and neural network) with three missingness mechanisms. Missing categorical features are encoded as their own category and missing numerical features are either mean-imputed or imputed using the complex iterative method mice (van Buuren and Groothuis-Oudshoorn 2010). The downstream predictive model is chosen among a regularized linear, tree, and a random forest model (using 5-fold cross-validation on the training data).

For mean-imputation, we compute the mean on the training data and use it to impute the missing values on both the training and testing data, in order to have the same imputation rule for the training and test set. For mice, however, the imputed value is neither a single value nor a simple function of the observed features. Hence, it is not possible to

Table 2 Difference in means and in pseudo-medians (with one-sided p-values) in out-of-sample accuracy from a t and Wilcoxon test applied to assess the impact of mice imputation on downstream accuracy. A negative impact means that mice reduces accuracy compared with mean-impute.

Signal Y	Missingness	Δ mean (p-value)	Δ pseudo-median (p-value)
	MAR	$-0.0093 (10^{-2})$	$-0.006 \ (< 10^{-22})$
Synthetic - Linear	NMAR	$-0.0113 \ (2 \cdot 10^{-6})$	$-0.0067 \ (< 10^{-22})$
	AM	0.0079(1)	0.0002 (0.84)
	MAR	-0.0138 (0.015)	$-0.0061 \ (< 10^{-22})$
Synthetic - NN	NMAR	$-0.0052 \ (0.074)$	$-0.003 \ (< 10^{-22})$
	AM	-0.0042 (0.028)	$-0.002 \ (7 \cdot 10^{-7})$
Real	Real	-0.0012 (0.37)	$-0.0026 \ (2 \cdot 10^{-3})$

guarantee exactly the same imputation rule for training and testing. Instead, we first impute the training set alone, and then impute the test set with the *imputed* training data. Since the test set is imputed with knowledge of the previously imputed training set, we can reasonably expect that the imputation on test data will mimic the strategy used in training, despite the black-box nature of the imputation method. We discuss alternative implementations in Appendix F.

Table 2 reports the output from paired t and Wilcoxon tests. Regarding difference in mean accuracy, we do not observe any statistical difference in downstream prediction accuracy between the two imputation methods in 5 out of the 7 cases. For the remaining 2 cases, we observe that the models trained after mice-imputation are marginally less accurate than those trained after mean-imputation. The difference in median accuracy leads to a similar conclusion, although mice-impute is more often (6 out of 7 cases) identified as less accurate with strong statistical significance (p-value $< 10^{-3}$).

3.4. Discussion: Limitations of Theorem 1

While Theorem 1 supports the use of simple imputation rules in practice (i.e., encoding missingness as a category for continuous features, and mean imputation for continuous ones), it is a population-level statement and applies to the large-sample regime. In particular, the asymptotic prediction rule $f_{\mu-imputed}$ is non-parametric. In practice, non-parametric methods might not scale to even moderate dimensions and one might favor parametric classes of predictors (instead of universally consistent learning algorithms). This can impact

the optimality of the resulting impute-then-regress model as well as the rate of convergence for finite n. Furthermore, while the missingness mechanism (MAR or NMAR) does not impact asymptotic Bayes optimality in Theorem 1, it can impact the estimation procedure with finite data. To illustrate these limitations, we consider a specific example where d=1 and the signal is generated according to a true linear model, $Y=w^*X_1+\varepsilon$, with ε an independent centered random noise with variance σ^2 .

If data is missing completely at random (MCAR), i.e., if M_1 is an independent Bernoulli variable with parameter p, then the Bayes optimal prediction rule is to predict w^*X_1 if $M_1 = 0$, and $w^*\mathbb{E}[X_1]$ otherwise. In other words, the optimal predictor corresponds to mean imputation followed by a linear model. Hence, mean-impute-then-regress with a downstream linear model is asymptotically consistent, while Theorem 1 only proves optimality when followed by a universally consistent model.

Alternatively, assume that the data is censored with $M_1 = 1$ if X_1 is greater or equal that its (1-p)th percentile, q_{1-p} . The Bayes optimal prediction rule is to predict w^*X_1 if $M_1 = 0$, and $w^*\mathbb{E}[X_1|X_1 \geq q_{1-p}]$ otherwise. Observe that this rule corresponds to μ -impute followed by a simple linear model. However, the imputed value should be $\mu = \mathbb{E}[X_1|X_1 \geq q_{1-p}]$, i.e., the conditional value-at-risk of X_1 at level 1-p, instead of the mean. Consequently, restricting our attention to mean-imputation followed by linear models would be suboptimal.

We illustrate this insight using data generated from this model (see Appendix E.1 for the detailed methodology) in Figure 1, which compares the normalized mean-square error (or R^2) of two impute-then-regress methods under the MCAR (blue lines) and censoring (orange lines) mechanisms: the first method imputes the mean, while the second optimizes the imputed value μ jointly with the downstream predictive model, using a method we develop in Section 5. In the left panel the downstream predictor is linear, while in the right panel it is selected via cross-validation among a linear model, tree, and random forest.

In the left panel all R^2 values converge quickly as n increases, because the downstream linear models can be trained with few samples. However, as described analytically, while imputing the mean and optimally selecting the imputed value are equivalent when the data is MCAR, mean-imputation followed by linear regression is sub-optimal when the data is censored. Using a more powerful downstream predictor (right panel) improves the predictive power of mean-impute-then-regress under censoring, but at the cost of many more

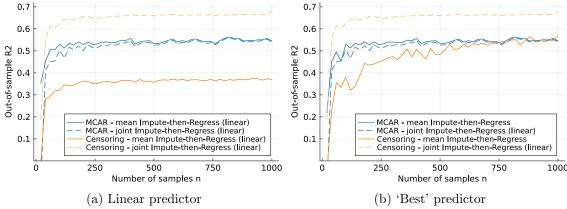


Figure 1 Convergence of out-of-sample R2 (normalized MSE) as a function of the number of training observations n for mean impute-then-regress (solid lines) vs. joint impute-then-regress (dash lines), when data is MCAR (blue) and censored (orange). The downstream predictive model is a linear model in the left panel and the best out of linear, tree, random forest in the right panel.

data samples. In contrast, using a more powerful downstream predictor does not improve the predictive power of optimal-impute-then-regress since a linear predictor already made this method optimal.

In addition, we observe in Figure 1 that the censored setting leads to higher accuracy than MCAR. Indeed, analytically, we find that the Bayes optimal mean square error in the former case is $\sigma^2 + p|w^*|^2 \operatorname{var}[X_1|X_1 \geq q_{1-p}]$ instead of $\sigma^2 + p|w^*|^2 \operatorname{var}[X_1]$ in the latter. This observation demonstrates that, although MAR is crucially needed for inference, it may be unnecessary and even counter-productive for prediction. We formalize this insight in the case of a single missing feature.

THEOREM 2. Consider two missingness mechanisms M_1 and M'_1 leading to the same proportion of missing entries $\mathbb{P}(M_1=1)=\mathbb{P}(M'_1=1)=p$. Further assume that, conditioned on $\mathbf{X}_{2:d}$, M'_1 is independent of Y and X_1 (MAR). Then the optimal prediction rule achieves a lower prediction error under M_1 than under M'_1 if and only if the following condition holds:

$$(1-p)^{2}\psi_{0}(\boldsymbol{X},\boldsymbol{X}) + p^{2}\psi_{1}(\boldsymbol{X}_{2:d},\boldsymbol{X}_{2:d}) + p(1-p)\psi_{0}(\boldsymbol{X}_{2:d},\boldsymbol{X}) - p(1-p)\psi_{1}(\boldsymbol{X},\boldsymbol{X}_{2:d}) \geq 0,$$

$$where \ \psi_{i}(A,B) = \mathbb{E}\left[\left(\mathbb{E}\left[Y|A\right] - \mathbb{E}\left[Y|B,M_{1}\right]\right)^{2}|M_{1} = i\right] \geq 0.$$

We discuss the condition in Theorem 2 at greater length in Appendix B, and illustrate it with the following two examples:

EXAMPLE 1 (PREDICTION BENEFITS FROM NMAR). Let X_1 be a Bernoulli random variable with parameter 1/2, and $Y = X_1$. We compare two missingness patterns: $M_1 = X_1$, and $M'_1 \perp X_1$, another Bernoulli random variable with parameter 1/2. Then, the optimal predictor under M_1 is $Y = X_1$ when $M_1 = 0$ and $Y = M_1 = 1$ when $M_1 = 1$, with empirical risk R = 0. Meanwhile, the Bayes-optimal predictor under M'_1 is $Y = X_1$ when $M'_1 = 0$ and Y = 1/2 when $M'_1 = 1$, with empirical risk R' = 1/8.

EXAMPLE 2 (PREDICTION BENEFITS FROM MAR). Let d=2, and let X_2 , U, V be three independent Bernoulli random variables with parameter 1/2. Define $X_1=X_2\mathbb{1}(U=0)+V\mathbb{1}(U=1)$ and let $Y=X_1$. We compare two missingness patterns: $M_1=U$, and M_1' an independent Bernoulli random variable with parameter 1/2. Then the Bayes-optimal learner under M_1 is X_1 when $M_1=0$ and 1/2 when $M_1=1$, with empirical risk R=1/8. In contrast, the Bayes-optimal learner under M_1' is X_1 when $M_1'=0$, and $X_2/2+1/4$ when $M_1'=1$, with empirical risk R'=3/32.

Though Theorem 1 guarantees the optimality of mean-impute-then-regress, we observe that optimality may rely on a data-hungry universally consistent downstream predictor, an inference-friendly MAR assumption on the missing data mechanism, or both. These limitations leave room for new methods. In the following sections, we seek to develop predictive models for partially missing data that perform well with limited samples and do not rely on the MAR assumption.

4. A Framework for Linear Regression with Missing Values

A natural question to ask is whether one could learn $\mathbb{E}[Y|M=m,o(X,M)=o(x,m)]$ directly, i.e., build a predictive model that (a) applies to the observed vectors o(X,M) directly, and (b) leverages information from the missingness pattern M and (c) is agnostic to the missing data mechanism.

4.1. Linear regression with missing values

Many learners, including linear models, cannot cope with the variable dimension of the vector o(x, m) by design, hence cannot be applied to observations with missing entries directly. To address this issue, we adopt a simple convention: when computing the output of a linear model, we omit the features that are missing. Formally, given a linear model

 $\boldsymbol{w} \in \mathbb{R}^d$, we define (and denote) the output of the linear model \boldsymbol{w} for the observation $\boldsymbol{x} \in \mathbb{R}^d$ and the missingness pattern $\boldsymbol{m} \in \{0,1\}^d$ as follows

$$\langle \boldsymbol{w}, \boldsymbol{x} \rangle_{\boldsymbol{m}} := \sum_{\substack{j=1 \ m_i=0}}^d w_j x_j = \sum_{j=1}^d w_j (1 - m_j) x_j.$$

Observe that the expressions above do not depend on the values of x_j for the features j that are missing $(m_j = 1)$. In other words, $\langle \boldsymbol{w}, \boldsymbol{x} \rangle_{\boldsymbol{m}}$ does not depend on the full vector \boldsymbol{x} but only on its observed coordinates $\boldsymbol{o}(\boldsymbol{x}, \boldsymbol{m})$. For concision, we will simply write $\langle \boldsymbol{w}, \boldsymbol{x} \rangle_{\boldsymbol{m}}$ (or later $f(\boldsymbol{x}, \boldsymbol{m})$), despite the fact that these expressions technically only depend on $\boldsymbol{o}(\boldsymbol{x}, \boldsymbol{m})$. This convention is also equivalent to assuming that missing entries are systematically imputed by 0.

In addition, as previously discussed, we would like our predictive model to be able to leverage the information contained in the missingness pattern directly. To do so, we allow the weights of our linear models to depend explicitly on the set of features available, i.e., we consider prediction rules of the form

$$f(\boldsymbol{x}, \boldsymbol{m}) = \langle \boldsymbol{w}(\boldsymbol{m}), \boldsymbol{x} \rangle_{\boldsymbol{m}} = \sum_{j=1}^{d} w_{j}(\boldsymbol{m})(1 - m_{j})x_{j}, \tag{4}$$

where the functions $w_j(\mathbf{m})$ are prescribed to a user-defined class \mathcal{F} . Given historical data $\{(\mathbf{m}_i, \mathbf{o}(\mathbf{x}_i, \mathbf{m}_i), y_i), i = 1, ..., n\}$, the functions $w_j(\cdot)$ can be computed by solving an empirical risk minimization problem

$$\min_{\boldsymbol{w}(\cdot)\in\mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell\left(y_i, \langle \boldsymbol{w}(\boldsymbol{m}_i), \boldsymbol{x}_i \rangle_{\boldsymbol{m}_i}\right), \tag{5}$$

for some loss function ℓ such as the squared error, $\ell(y,z) = (y-z)^2$.

4.2. A hierarchy of adaptive linear regression models

We now derive a hierarchy of linear models, according to how the functions $w_j(\mathbf{m})$ in (4) depend on the missingness pattern, borrowing ideas from the multi-stage adaptive optimization literature. We first consider two extreme special cases for \mathcal{F} , namely the fully adaptive and static case.

Fully adaptive regression. The fully adaptive case corresponds to the situation where we consider a different linear model for each potential missingness patterns m. Formally, each function $w_i(m)$ is of the form

$$w_j(oldsymbol{m}) = \sum_{oldsymbol{m}' \in \{0,1\}^d} w_{j,m'} \mathbf{1}(oldsymbol{m} = oldsymbol{m}'), \quad ext{with} \quad \mathbf{1}(oldsymbol{m} = oldsymbol{m}') := egin{cases} 1 & ext{if } oldsymbol{m} = oldsymbol{m}', \ 0 & ext{otherwise.} \end{cases}$$

Oberve that, since m is a binary vector, $w_j(m)$ can be considered as an order-d polynomial in m. Indeed, we have

$$\mathbf{1}(\boldsymbol{m} = \boldsymbol{m}') = \prod_{j=1}^{d} (1 - (m_j - m_j')^2) = \prod_{j=1}^{d} (1 - m_j - m_j' + 2m_j m_j').$$

This approach is equivalent to partitioning the training dataset according to the set of available features and train a linear model on each part separately. There are two major drawbacks in this approach: First, it treats each missingness pattern separately, hence substantially reducing the number of observations available to fit each model. Second, there can be as many as 2^d potential missingness patterns, i.e, 2^d models to be trained, rendering the fully adaptive approach potentially intractable. Yet, often in practice, only $d' \ll d$ covariates might be subject to missingness and the actual number of patterns to consider can be substantially smaller.

Static regression. On the opposite side of the spectrum, we can consider a static model w(m) = w which does not depend on m. This is equivalent to fitting a linear model on a full dataset where missing values are replaced by 0. Note that this is not equivalent to applying mean-impute on the data before training a linear model. By imputing missing values with a 0, a missing feature effectively does not contribute to the output of the model, while any non-zero value would have affected the final prediction.

Between these two extremes, one can consider specific functional forms for w(m) such as linear or polynomial functions that could be use to trade-off adaptivity and tractability.

Affinely adaptive regression. Affine policies are a successful and often-used tool in adaptive optimization, as they are typically more powerful than a static policy but more tractable than a fully adaptive one (Ben-Tal et al. 2004, Bertsimas and Goyal 2012). An affinely adaptive linear model takes the form

$$w_{j}^{\text{affine}}(\boldsymbol{m}) = w_{0,j} + \sum_{j'=1}^{d} W_{jj'} m_{j'},$$

or $\boldsymbol{w}_{j}^{\text{affine}}(\boldsymbol{m}) = \boldsymbol{w}_{0} + \boldsymbol{W}\boldsymbol{m}$ with matrix notations. Here, \boldsymbol{w}_{0} corresponds to a baseline model to be used when all features are present and $W_{jj'}$ represents the linear correction to apply to the $w_{0,j}$ whenever feature j' is missing. For a given observation $(\boldsymbol{o}(\boldsymbol{x},\boldsymbol{m}),\boldsymbol{m})$, a prediction is obtained by computing $\langle \boldsymbol{w}_{0} + \boldsymbol{W}\boldsymbol{m}, \boldsymbol{x} \rangle_{\boldsymbol{m}} = \sum_{j} w_{0j}(1-m_{j})x_{j} + \sum_{j,k} W_{jk}m_{k}(1-m_{j})x_{j}$. Accordingly, fitting \boldsymbol{w}_{0} and \boldsymbol{W} is equivalent to fitting a linear regression model over the $d+d^{2}$ features of the form $(1-m_{j})x_{j}$, for $j=1,\ldots,d$ (zero-imputed dataset) and $m_{k}(1-m_{j})x_{j}$ for $j,k=1,\ldots,d$.

Polynomially adaptive regression. In addition to affine functions, polynomial decision rules have been theoretically and empirically investigated in the adaptive multi-stage optimization literature (see, e.g., Bertsimas et al. 2009, 2011). Similarly, in our setting, one could consider weights that are order-t polynomials, for some $t \in \{1, ..., d\}$. In this case, each weight function $w_j(\mathbf{m})$ can be viewed as a linear function in the monomials of the form $\prod_{j \in \mathcal{J}} m_j$, with $\mathcal{J} \subseteq \{1, ..., d\}$, $|\mathcal{J}| \le t$. Hence, $f(\mathbf{x}, \mathbf{m})$ can be seen as a linear function in the $\mathcal{O}(d^{t+1})$ variables of the form $x_{j'}(1-m_{j'})\prod_{j \in \mathcal{J}} m_j$ (and fitted as such).

Finitely adaptive regression. Another way to balance the trade-off between expressiveness of the adaptive model and tractability is finite adaptability. Formally, we can partition the space of all possible missingness patterns $\mathcal{M} \subseteq \{0,1\}^d$ into Q disjoint subsets $\{\mathcal{M}_q\}_{q=1}^Q$ such that $\mathcal{M} = \bigcup_{q=1}^Q \mathcal{M}_q$ and define a distinct linear regression model for each \mathcal{M}_q , i.e., train a model of the form $\mathbf{w}(\mathbf{m}) = \sum_{q=1}^Q \mathbf{w}_q \mathbf{1}(\mathbf{m} \in \mathcal{M}_q)$. As in the fully adaptive case, one can show that the indicator functions $\mathbf{1}(\mathbf{m} \in \mathcal{M}_q)$ are polynomial functions in \mathbf{m} . Hence, finitely adaptive regression can be seen as a special case of polynomially adaptive regression, where monomials are introduced dynamically.

The main difficulty of a finitely adaptive approach is in choosing the partition $\{\mathcal{M}_q\}_{q=1}^Q$. We propose an greedy heuristic that simultaneously learns the partition $\{\mathcal{M}_q\}_{q=1}^Q$ and the appropriate regression models \boldsymbol{w}_q based on recursive partitioning (Algorithm 1 in Appendix C). At each iteration, we consider splitting each subset, denoted \mathcal{M}_q , into two subsets $\mathcal{M}_q^{j,0} := \mathcal{M}_q \cap \{\boldsymbol{m} : m_j = 0\}$ and $\mathcal{M}_q^{j,1} 1 := \mathcal{M}_q \cap \{\boldsymbol{m} : m_j = 1\}$ for all features j, and choose the feature j^* that leads to the highest reduction in empirical risk. To prevent overfitting, we add different stopping criteria that make further splitting inadmissible. For instance, we can impose a limit on the minimum number of samples per leaf, on the total depth of the resulting partitioning tree, or only allow splits that sufficiently reduce the in-sample error.

4.3. Finite-sample generalization bounds for adaptive linear regression

Intuitively, choosing a more complex class of functions for our adaptive weights $w_j(\mathbf{m})$ can increase predictive accuracy, because it can model more complex relationships, but is also more prone to overfitting due to the increased number of parameters to calibrate. We formalize this trade-off in this section, by deriving finite-sample bounds for adaptive linear regression models with polynomial weights. To conduct our analysis, we adopt a similar theoretical setting as Le Morvan et al. (2020).

Assumption 1. We have $Y = f^*(\mathbf{X}, \mathbf{M}) + \varepsilon$ where, conditional on (\mathbf{X}, \mathbf{M}) , ε is a centered noise with variance σ^2 and $f^*(\mathbf{X}, \mathbf{M})$ is of the following form

$$f^{\star}(\boldsymbol{X}, \boldsymbol{M}) = \sum_{\boldsymbol{m} \in \{0,1\}^d} \left(\sum_{j=1}^d w_{j,m}^{\star} (1 - M_j) X_j \right) \mathbf{1}(\boldsymbol{M} = \boldsymbol{m}),$$

Furthermore, we have $||f^*||_{\infty} \leq L$.

In the words of Section 4.2, Assumption 1 states that the ground truth is a fully adaptive linear model. We refer to Le Morvan et al. (2020, proposition 4.1) for specific conditions on the dependency between X and Y and on the missingness mechanisms that lead to Assumption 1. As in Györfi et al. (2002, chapter 13), we consider a truncated version of our linear regression estimate, defined as $T_L f(x) := f(x)$ if $|f(x)| \le L$, L if f(x) > L, and -L if f(x) < -L. With this assumption, we obtain the following result:

THEOREM 3. Consider a function a class \mathcal{F} and adaptive linear regression models of the form (4) with $w_j(\mathbf{m}) \in \mathcal{F}$. Denote \hat{f}_n the ordinary least square estimator obtained from a dataset of size n and assume that fitting \hat{f}_n is equivalent to fitting a linear model with $p(\mathcal{F})$ coefficients. Under Assumption 1, there exists a universal constant c > 0 such that

$$\mathbb{E}\left[\left(Y - T_L \hat{f}_n(\boldsymbol{X}, \boldsymbol{M})\right)^2\right] \le \sigma^2 + 8b(\mathcal{F}) + c \max\{\sigma^2, L\} \frac{1 + \log n}{n} p(\mathcal{F}),$$

where $b(\mathcal{F})$ is an upper-bound on the estimation bias, $\min_{f \in \mathcal{F}} \mathbb{E}\left[(f^*(\boldsymbol{X}, \boldsymbol{M}) - f(\boldsymbol{X}, \boldsymbol{M}))^2 \right]$ (hence depends on \mathcal{F} and d but is independent of n). Formulas/bounds for the constants $p(\mathcal{F})$ and $b(\mathcal{F})$ are given in Table 3.

Proof of Theorem 3 By decomposing $Y = f^*(\boldsymbol{X}, \boldsymbol{M}) + \varepsilon$, we obtain

$$\mathbb{E}\left[\left(Y - T_L \hat{f}_n(\boldsymbol{X}, \boldsymbol{M})\right)^2\right] = \mathbb{E}\left[\left(f^{\star}(\boldsymbol{X}, \boldsymbol{M}) - T_L \hat{f}_n(\boldsymbol{X}, \boldsymbol{M})\right)^2\right] + \mathbb{E}\left[\varepsilon^2\right].$$

\mathcal{F} : class for $w_j(\boldsymbol{m})$	$b(\mathcal{F})$	$p(\mathcal{F})$
Static	$\mathcal{O}\left(d ight)$	d
Affine	$\mathcal{O}\left(d^2 ight)$	$d+d^2$
Order- t polynomial	$\mathcal{O}\left(\frac{d^{t+1}}{(t+1)^{3(t+1)}}\right)$	$\mathcal{O}(d^{t+1})$
Fully adaptive	0	$d2^d$

Table 3 Formula/bounds for the constants $b(\mathcal{F})$ and $p(\mathcal{F})$ involved in the finite-sample guarantees in Theorem 3 for different adaptive linear regression models in our hierarchy.

According to Györfi et al. (2002, theorem 11.3), the first term on the right-hand side can be bounded by

$$8\inf_{f\in\mathcal{F}}\mathbb{E}\left[\left(f^{\star}(\boldsymbol{X},\boldsymbol{M})-f(\boldsymbol{X},\boldsymbol{M})\right)^{2}\right]+c\max\{\sigma^{2},L\}\frac{1+\log n}{n}p(\mathcal{F}),$$

while the second term is bounded by σ^2 .

To bound $\inf_{f \in \mathcal{F}} \mathbb{E}\left[(f^*(\boldsymbol{X}, \boldsymbol{M}) - f(\boldsymbol{X}, \boldsymbol{M}))^2 \right]$, it is sufficient to bound $\mathbb{E}\left[(f^*(\boldsymbol{X}, \boldsymbol{M}) - f(\boldsymbol{X}, \boldsymbol{M}))^2 \right]$ for some $f \in \mathcal{F}$. In particular, defining $f(\boldsymbol{x}, \boldsymbol{m})$ as the order- $f(\boldsymbol{x}, \boldsymbol{M})$ and $f(\boldsymbol{x}, \boldsymbol{m})$ and $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ and $f(\boldsymbol{x}, \boldsymbol{m})$ and $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ and $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ and $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ and $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ and $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ and $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ and $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ and $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ and $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ and $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ and $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ and $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ are $f(\boldsymbol{x}, \boldsymbol{m})$ and $f(\boldsymbol{x$

$$\mathbb{E}\left[|f^{\star}(\boldsymbol{X},\boldsymbol{M}) - f(\boldsymbol{X},\boldsymbol{M})|^{2}\right] = \mathcal{O}\left(\frac{d^{t+1}}{(t+1)^{3(t+1)}}\right).$$

Intuitively, Theorem 3 shows that, as we consider higher-order polynomials as adaptive rules, the number of parameters to calibrate, $p(\mathcal{F})$ grows exponentially but the bias term (provided that the ground truth corresponds to a fully adaptive model as stated in Assumption 1) decays super-exponentially in t.

4.4. Implementation details

Our adaptive linear regression models can be viewed as linear regression models over an extended set of $p(\mathcal{F})$ features. To mitigate the issue of overfitting, we consider an ℓ_1 - ℓ_2 -penalized version of the empirical risk minimization problem (5), commonly referred to as ElasticNet (see Hastie et al. 2001, section 3.4.2) and implemented in the package glmnet. The ElasticNet formulation involves a parameter λ controlling the amount of regularization. As supported by intuition and theory, the more data is available, the less regularization is needed. However, in our case, many of the features are sparse binary

features (e.g., m_j). For each of these features, the effective number of samples available to calibrate its coefficient value is not n but the number of samples for which it is non-zero (e.g., $\sum_{i \in [n]} m_{ij} \leq n$). Accordingly, we apply a different λ value for each feature, proportionally to the missingness frequency of each feature.

5. Extension to Adaptive Non-Linear Regression

We now extend the adaptive linear regression framework developed in Section 4 to generic non-linear models. To deal with inputs o(x,m) of varying dimension, we proposed in the linear case to set the missing features to zero. This convention appears natural for linear models since setting a variable to zero effectively implies that this variable does not contribute to the output. However, this convention is hard to generalize to other models (e.g., tree-based models) for which the impact of zero-imputation on the output is not predictable. Therefore, to extend our adaptive regression framework, we first show a connection, in the linear case, between adaptive linear models and joint impute-then-regress strategies and then propose a heuristic to perform joint impute-then-regress with non-linear models.

5.1. Connection between adaptive regression and optimal impute-then-regress

We consider a special case of affinely adaptive linear regression where all the regression coefficients are static except for the intercept (i.e., a feature x_j that is constant, equal to 1, and never missing), which depends on the missingness pattern in an affine way, i.e., $f(\boldsymbol{x}, \boldsymbol{m}) = b(\boldsymbol{m}) + \langle \boldsymbol{w}, \boldsymbol{x} \rangle_{\boldsymbol{m}}$, where $b(\boldsymbol{m}) = b_0 + \sum_j b_j m_j$. In this case, the prediction function is

$$f(\boldsymbol{x}, \boldsymbol{m}) = b_0 + \sum_{j=1}^{d} (w_j (1 - m_j) x_j + b_j m_j) = b_0 + \sum_{j=1}^{d} w_j \left((1 - m_j) x_j + m_j \frac{b_j}{w_j} \right).$$

In other words, a static regression model with affinely adaptive intercept can be viewed as imputing $\mu_j := b_j/w_j$ for feature j whenever it is missing, and then applying a linear model \boldsymbol{w} . The key difference with standard impute-then-regress strategies, however, is that the vector of imputed values $\boldsymbol{\mu}$ and the linear model \boldsymbol{w} are computed simultaneously, instead of sequentially, hence leading to greater predictive power². Note that this family of models correspond to the affine approximation in Le Morvan et al. (2020, definition 4.1).

² Note that our algebraic manipulation, and the resulting interpretation, is valid only if $w_j \neq 0$. If $w_j = 0$ and $b_j \neq 0$, it means that feature j is not a strong predictor of the outcome variable y but the fact that it is missing, m_j , is.

In the simple case where there is only one feature X_1 , this family of models would learn the rule $w_1(X_1(1-M_1) + \mu_1 M_1)$ with

$$\mu_1 = \frac{1}{w_1} \mathbb{E}[Y|M_1 = 1] = \frac{\mathbb{E}[Y|M_1 = 1]\mathbb{E}[X_1^2|M_1 = 0]}{\mathbb{E}[YX_1|M_1 = 0]}.$$

Compared with classical imputation methods, we observe that the imputed value does not only depend on the distribution of X_1 on the samples where it is observed $(M_1 = 0)$. Rather, (a) it depends on the target variable Y, and (b) it involves observations for which X_1 is missing $(M_1 = 1)$. In particular, if Y satisfies a linear relationship $Y = w_1^*X_1$, then $\mu_1 = \mathbb{E}[X_1|M_1 = 1]$. In contrast, standard mean-imputation would select $\mu_1 = \mathbb{E}[X_1|M_1 = 0]$. In the same vein, we can interpret adaptive linear regression models as jointly learning an imputation rule and a predictive model, where more complex adaptive rules for the intercept can be interpreted as more sophisticated imputation rules. We will use this interpretation to generalize our adaptive linear regression framework to non-linear predictors in the following section.

Finally, let us observe that static regression models with an affinely adaptive intercept are very easy to compute in practice. They correspond to a simple linear regression model over 2d+1 variables, the d coordinates of \boldsymbol{x} (with missing values imputed as 0) along with the d coordinates of \boldsymbol{m} , as well as an intercept term b_0 .

5.2. Heuristic method for joint impute-and-regress

We now propose an iterative heuristic to jointly optimize for a simple imputation model μ and a downstream predictive model f. We initialize μ with the mean of each variable, i.e., mean-imputation. At each iteration, we train the predictive model on the μ -imputed data, X^{μ} . Then, for a fixed model f, we update the vector of imputed values μ so as to decrease the prediction error (e.g., mean squared error for regression, AUC for classification). For non-linear (or even non-parametric) models, minimizing $\mu \mapsto \operatorname{error}(Y, f(X^{\mu}))$ may not be tractable so we use a local search heuristic (or cyclic coordinate update heuristic) instead. For each coordinate $j \in [p]$, we update μ_j by increments of $\pm \sigma_j$ where σ_j is the standard error on the mean of X_j . As stopping criteria, we impose a limit on the total number of iterations (in our implementation, 20), on the number of coordinate updates at each iteration (10), and on the minimum relative improvement in prediction error (10⁻⁴). Pseudo-code is given in Algorithm 2 in Appendix C.

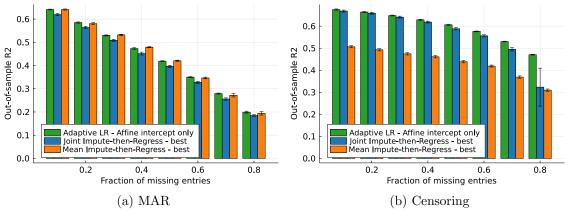


Figure 2 Out-of-sample R^2 of mean-impute-then-regress, joint impute-then-regress, and optimal μ -impute-then-regress on synthetic data with linear signal Y.

5.3. Evaluation of joint impute-and-regress strategies on synthetic data

We now present numerical results to evaluate the benefit of joint impute-then-regress strategies. In order to illustrate the relevance of joint-impute-then-regress and the validity of our heuristic, we use synthetic data generated following the methodology presented in Appendix E.1. In total, this methodology generates instances with 2 different models for the relationship between Y and X (linear or neural network) and 2 missingness mechanisms (missing completely at random and censoring). We also vary the sample size and the proportion of missing entries.

Figure 2 compares the out-of-sample R^2 of several methods in settings where Y is generated according to a linear model and data is missing completely at random (resp. censored) on the left (resp. right) panel. Figure 3 reports the same results on instances where Y is generated according to a neural network model. Both figures compare mean impute-then-regress with the heuristic for joint impute-then-regress presented in Section 5.2. For each of them, the downstream predictive model is chosen via 5-fold cross-validation among linear, tree, and random forest ('best'). As a point of comparison for our heuristic, for linear Y in Figure 2, we also report the performance of the optimal μ -impute-then-regress model from Section 5.1.

While competitive in MAR settings, we observe that mean impute-then-regress methods provides suboptimal predictive power whenever the data is censored. These results highlight the key deficiency of naive impute-then-regress strategies: they hide the missingness indicator to the downstream predictive model, hence losing potentially predictive information. On the contrary, our joint impute-then-regress heuristic is one of the best performing

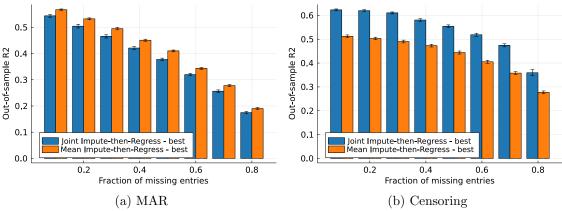


Figure 3 Out-of-sample \mathbb{R}^2 of mean-impute-then-regress and joint impute-then-regress on synthetic data with signal Y defined as the output function of a two-layer neural network.

methods, in both MAR and censored settings. The performance of our heurisite is comparable with that of optimal μ -impute-then-regress in the linear case, which demonstrates the effectiveness of our proposed heuristic. In addition, our simple heuristic procedure is versatile and can be used with any predictive model.

Table 4 additionally reports the performance of an impute-then-regress strategy with a sophisticated imputation rule called mice (van Buuren and Groothuis-Oudshoorn 2010) and the "Missing Incorporated in Attribute" (MIA) method of Twala et al. (2008)—implemented via $\pm \infty$ imputation of the missing entries as described in Josse et al. (2019, remark 5). We also report the performance of one adaptive linear regression model (Section 4), chosen among static with affine intercept, affine, or finite models via 5-fold cross validation on the training set ('Adaptive LR - best'). We still observe that sequential impute-then-regress strategies experience strong performance deterioration when data is not missing at random, compared to our adaptive linear regression and joint impute-then-regress models. We also make two striking observations. First, when the data is not missing at random, the predictive power (as captured by R^2) can be higher than in the MCAR case, hence corroborating our theoretical derivations in Section 3.4. Second, we observe that our adaptive linear regression models, although linear, perform very well in our experiments, even when the true signal is generated according to a neural network model.

6. Numerical experiments on real data

Finally, we evaluate the performance of the adaptive linear regression models proposed in Section 4 (static with affine intercept, affine, and finite) and the joint impute-then-regress heuristic from Section 5.2 on real-world data, as described in Appendix E.2. Our

Method	MC	CAR	Censoring		
	Linear	NN	Linear	NN	
Adaptive LR - best	0.473 (0.003)	0.434 (0.003)	0.604 (0.001)	0.607 (0.002)	
Joint Impute-then-Regress - best	0.414 (0.003)	0.383 (0.003)	0.569 (0.011)	0.543 (0.003)	
Mean Impute-then-Regress - best	0.433 (0.003)	$0.409 \ (0.002)$	0.434 (0.002)	$0.433 \ (0.002)$	
mice Impute-then-Regress - best	0.494 (0.004)	0.444 (0.003)	0.350 (0.004)	0.339 (0.004)	
CART MIA	0.262 (0.003)	0.244 (0.003)	0.462 (0.002)	0.452 (0.002)	

Table 4 Average out-of-sample \mathbb{R}^2 (and standard error) for each method on synthetic datasets, where Y is generated according to a linear or a neural network model, and the data is either missing completely at random or censored. Results are averaged over 50 different training sizes, 8 missingness level, and 10 random training/test set splits.

experimental benchmark comprises both synthetic (linear and neural network) signals and real signals. For synthetic signals, we control the dependency between Y and X, M so that the missingness can be missing at random (MAR), not missing at random (NMAR), or adversarially missing (AM), as explained in Appendix E.2.2.

Figure 4 displays the average out-of-sample performance for our adaptive linear regression models (left panel) and our joint impute-then-regress heuristic (right panel). For adaptive linear regression, we observe that the static with affine intercept and affine variants achieve the best and comparable performance, while finite adaptive is often the worst performing method. By cross-validating the degree of adaptivity, the 'best' variant successfully achieves the best performance overall. For the joint impute-then-regress heuristic, we surprisingly observe very strong performance from using a linear downstream predictive model, even when the true signal is non-linear, suggesting that our heuristic procedure might be more favorable to models whose output depends continuously on the input variables.

We now compare the accuracy of the best adaptive linear regression and joint impute-then-regress model with a mean-impute-then-regress model (with the downstream predictive model chosen via cross-validation). As benchmarks, we also compare to a "complete feature" regression model (i.e., using only features that are never missing) and, for synthetic signal, an "oracle" model, which has access to the fully observed dataset x_{full} and m. As displayed in Figure 5, we first observe that the complete feature regression model performs significantly worse than all other methods, emphasizing the danger of systematically discarding missing features in practice. Note that this conclusion holds despite the fact that features are correlated. Second, we observe that, while competitive under MAR, the

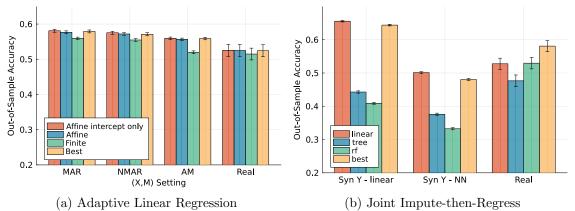


Figure 4 Performance of adaptive linear regression (left panel) and joint impute-then-regress models (right panel) on real-world design matrix X.

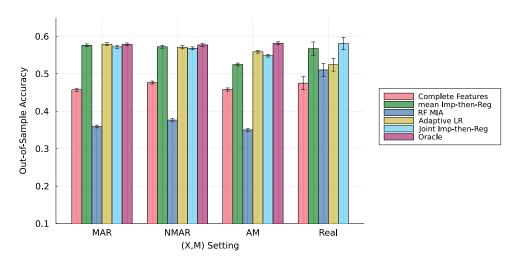


Figure 5 Comparison of adaptive linear regression and joint impute-then-regress methods vs. mean-impute-then-regress on real-world design matrix X. We also compare to two extremes: the "Oracle" which has access to the fully observed data and the "Complete Feature" regression which regresses of features that are never missing only.

performance of mean impute-then-regress deteriorates as missingness becomes adversiarilly missing (AM), compared with both the oracle and our adaptive/joint impute-then-regress strategies. Again, these results highlight that applying imputation and regression sequentially, although potentially optimal when MAR (c.f. Theorem 1), cannot appropriately leverage the predictive power of missingness itself. Nonetheless, we should mention that on real signals Y, mean impute-then-regress is the second best performing method after joint impute-then-regress, which could be explained by the fact that the real-world data is closer to MAR than AM.

We further support this finding in Figure 6 in appendix, where we report out-of-sample accuracy for each synthetic signal setting, as a function of the fraction of missing features contributing to the signal. We observe that mean-impute-then-regress methods achieve comparable accuracy as the oracle, adaptive linear regression, and joint-impute-then-regress models in the MAR and NMAR setting. However, they experience a significant drop in accuracy in the AM setting, which grows as the proportion of missing features $k_{missing}/k$ increases.

Alternatively, for each unique dataset, we count how often the adaptive linear regression model (resp. joint Impute-then-regress model) outperforms mean-impute-then-regress method over 10 random training/test set splits and display the density for this percentage of "wins" in Figure 7. The trend is clear: as the missingness mechanisms departs further away from the MAR assumption, adaptive models improve more often over impute-then-regress. Comparing these profiles with those obtained on the real Y experiments (Figure 8), we observe that the benefit from our method is not as obvious and systematic as in the semi-synthetic AM case, suggesting that, in our library of real-world datasets, the data is more often missing at random than adversially missing.

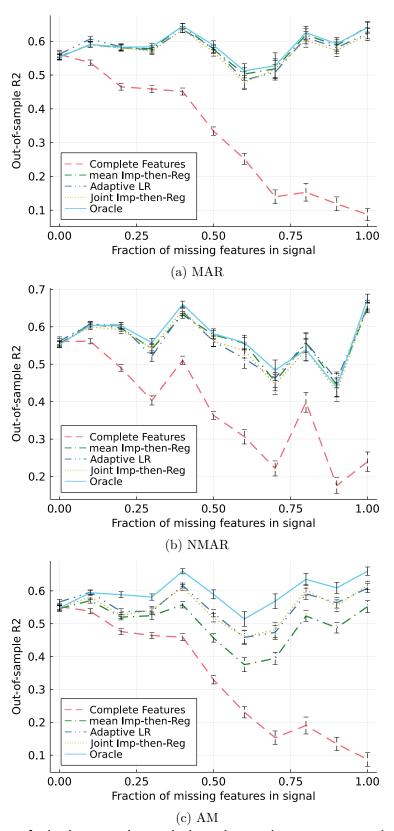


Figure 6 Comparison of adaptive regression methods vs. impute-then-regress on synthetic data, as $k_{missing}$ increases. We also compare to two extremes: the "Oracle" which has access to the fully observed data and the "Complete Feature" regression which regresses of features that are never missing only.

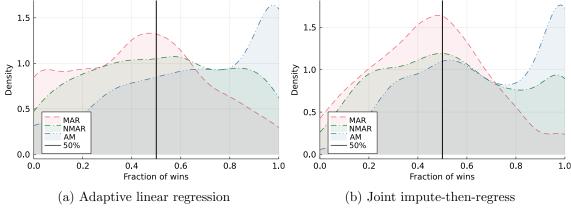


Figure 7 Frequency of "wins" from adaptive models vs. mean-impute-then-regress ones.

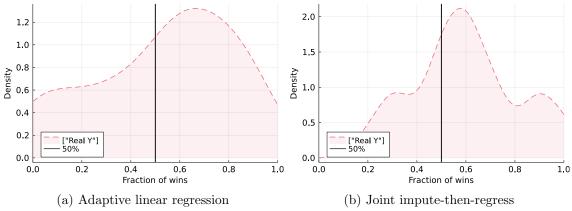


Figure 8 Frequency of "wins" from adaptive models vs. mean-impute-then-regress ones.

7. Conclusion

Statistical inference and prediction are two distinct but intertwined functions of statistical models (Shmueli et al. 2010). In inference settings, data imputation, in particular multiple data imputation, is the gold standard for dealing with missing information. In this paper, we investigate its relevance for predictive tasks. In Section 3, we provide both theoretical and empirical evidence to support the use of simple but effective imputation rules, namely mean imputation for continuous variables and encoding missingness as a category for categorical ones. However, these results do not account for the amount of data needed to achieve the best performance. Accordingly, we develop adaptive linear regression models and a joint impute-then-regress heuristic in Sections 4 and 5 that achieve higher predictive power, especially in NMAR settings. Our extensive numerical results on synthetic, semi-synthetic, and real datasets also raise interesting questions for future research, regarding

the relevance and applicability of the Missing at Random assumption and the ability to generate synthetic yet realistic datasets with missing entries.

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Appendix A: Proof of Theorem 1

Proof Since the downstream predictive model is trained after μ -imputation, the learner is trained not on $(\boldsymbol{o}(\boldsymbol{X}, M_1), M_1)$ but on its imputed version \boldsymbol{X}^{μ} . Accordingly, asymptotically, $f_{\mu-impute}(\boldsymbol{x}) = \mathbb{E}[Y|\boldsymbol{X}^{\mu} = \boldsymbol{x}]$. We now relate the conditional expectation of $Y|X_1^{\mu} = x_1^{\mu}, \boldsymbol{X}_{2:d} = \boldsymbol{x}_{2:d}$ with those of $Y|M_1 = 1, \boldsymbol{X}_{2:d} = \boldsymbol{x}_{2:d}$ and $Y|M_1 = 0, X_1 = x_1^{\mu}, \boldsymbol{X}_{2:d} = \boldsymbol{x}_{2:d}$.

For random variables Z_1, Z_2 , we denote $g_{Z_1}(z_1)dz_1$ the distribution function of Z_1 and $g_{Z_1}(z_1|Z_2=z_2)dz_1$ the distribution function of $Z_1|Z_2=z_2$.

We condition on the event $\{X_{2:d} = x_{2:d}\}$ for some $x_{2:d}$ such that $g_{X_{2:d}}(x_{2:d}) > 0$. All our reasoning is conditioned on $\{X_{2:d} = x_{2:d}\}$, e.g., all distributions/probabilities are conditional distributions/probabilities, but we omit the dependency on $x_{2:d}$ for simplicity. We also denote $\mu := \mu(x_{2:d})$.

The joint density for (X_1, M_1, X_1^{μ}) is $\left(\mathbf{1}_{m_1=1}\mathbf{1}_{x_1^{\mu}=\mu} + \mathbf{1}_{m_1=0}\mathbf{1}_{x_1^{\mu}=x_1}\right)g_{(X_1,M_1)}(x_1,m_1)dx_1^{\mu}dx_1dm_1$. By integrating over (X_1, M_1) , we obtain the density of X_1^{μ} :

$$h(x_1^{\mu})dx_1^{\mu} := \mathbb{P}(M_1 = 1)\mathbf{1}_{x_1^{\mu} = \mu}dx_1^{\mu} + g_{(X_1, M_1)}(x_1^{\mu}, 0)dx_1^{\mu}.$$

Note that

$$h(x_1^{\mu})dx_1^{\mu} = \begin{cases} g_{(X_1,M_1)}(x_1^{\mu},0)dx_1^{\mu} & \text{if } x_1^{\mu} \neq \mu, \\ \mathbb{P}(M_1 = 1) + g_{(X_1,M_1)}(\mu,0)dx_1^{\mu} & \text{if } x_1^{\mu} = \mu. \end{cases}$$

Furthermore, let us denote $h(y, x_1^{\mu})$ the joint density of (Y, X_1^{μ}) . Since the joint density for (Y, X_1, M_1, X_1^{μ}) is $g_Y(y|X_1 = x_1, M_1 = m_1) \left(\mathbf{1}_{m_1=1}\mathbf{1}_{x_1^{\mu}=\mu} + \mathbf{1}_{m_1=0}\mathbf{1}_{x_1^{\mu}=x_1}\right) g_{(X_1, M_1)}(x_1, m_1) dy dx_1^{\mu} dx_1 dm_1$, we have

$$h(y,x_1^\mu)dydx_1^\mu = \mathbf{1}_{x_1^\mu = \mu}g_Y(y|M_1 = 1)\mathbb{P}(M_1 = 1)dydx_1^\mu + g_Y(y|X_1 = x_1^\mu, M_1 = 0)g_{(X_1,M_1)}(x_1^\mu,0)dydx_1^\mu + g_Y(y|X_1 = x_1^\mu, M_2 = 0)g_{(X_1,M_1)}(x_1^\mu,0)dydx_1^\mu + g_Y(y|X_1 = x_1^\mu, M_2 = 0)g_{(X_1,M_2)}(x_1^\mu,0)dydx_1^\mu + g_Y(y|X_1 = x_1^\mu, M_2 = 0)g_{(X_1,M_2)}(x_1^\mu,0)$$

Accordingly,

$$\begin{split} \int yh(y,x_1^\mu)dy &= \mathbf{1}_{x_1^\mu = \mu} \mathbb{P}(M_1 = 1) \int yg_Y(y|M_1 = 1)dy + g_{(X_1,M_1)}(x_1^\mu,0) \int yg_Y(y|X_1 = x_1^\mu,M_1 = 0)dy \\ &= \mathbf{1}_{x_1^\mu = \mu} \mathbb{P}(M_1 = 1)\mathbb{E}[Y|M_1 = 1] + g_{(X_1,M_1)}(x_1^\mu,0)\mathbb{E}[Y|M_1 = 0,X_1 = x_1^\mu]. \end{split}$$

All together, distinguishing the case where (X_1, M_1) is continuous/discrete and denoting

$$\alpha = \frac{\mathbb{P}(M_1 = 1)}{\mathbb{P}(M_1 = 1) + \mathbb{P}(X_1 = \mu, M_1 = 0)},$$

we obtain

$$\mathbb{E}[Y|X_1^{\mu} = x_1^{\mu}] = \begin{cases} \mathbb{E}[Y|X_1 = x_1^{\mu}, M_1 = 0] & \text{if } x_1^{\mu} \neq \mu, \\ \alpha \, \mathbb{E}[Y|M_1 = 1] + (1 - \alpha) \, \mathbb{E}[Y|X_1 = \mu, M_1 = 0] & \text{if } x_1^{\mu} = \mu. \end{cases}$$

Appendix B: Proof of Theorem 2

The quantities $\psi_i(A, B)$ in Theorem 2 measure the distance between $\mathbb{E}[Y|A]$ and $\mathbb{E}[Y|B, M_1]$ conditional on $M_1 = i$. In other words, these quantities compare the predictive power (on Y) of feature set A and feature set $\{B, M_1\}$. We note from the signs in the condition in Theorem 2 that a sufficient condition for the NMAR setting to yield higher predictive power is $\mathbb{E}\left[\left(\mathbb{E}[Y|X] - \mathbb{E}[Y|X_{2:d}, M_1]\right)^2 | M_1 = i\right] = 0$, corresponding to the case where M_1 is a perfect substitute for X_1 . This condition is not necessary since the first three terms can be strictly positive: in this case, NMAR can lead to higher predictive power as long as replacing the value X_1 with the fact that it is missing preserves enough information about the value of Y.

While data missing adversarially or not at random can make inference difficult or impossible, in prediction the *opposite* can be true. Theorem 2 shows that the relevance of assuming mechanisms for missing data methods is reduced in prediction as compared to inference. This insight is valuable because missing data mechanisms are inherently unobservable; a key property of the adaptive methods we develop in Sections 4 and 5 is their good predictive performance regardless of the missing data mechanism. Before proposing these methods, however, we first study the behavior of standard impute-then-regress methods.

Proof of Theorem 2 Let R(R') designate the optimal empirical risk under missingness $M_1(M'_1)$.

$$R = (1 - p)\mathbb{E}\left[(Y - \mathbb{E}\left[Y | \boldsymbol{X}, M_1\right])^2 | M_1 = 0 \right] + p\mathbb{E}\left[(Y - \mathbb{E}\left[Y | \boldsymbol{X}_{2:d}, M_1\right])^2 | M_1 = 1 \right],$$

$$R' = (1 - p)\mathbb{E}\left[(Y - \mathbb{E}\left[Y | \boldsymbol{X}, M_1'\right])^2 | M_1' = 0 \right] + p\mathbb{E}\left[(Y - \mathbb{E}\left[Y | \boldsymbol{X}_{2:d}, M_1'\right])^2 | M_1' = 1 \right].$$

Because M'_1 is independent of Y given $X_{2:d}$, we can write:

$$\begin{split} R' &= (1-p)\mathbb{E}\left[(Y - \mathbb{E}\left[Y|\boldsymbol{X}\right])^2 | M_1' = 0 \right] + p\mathbb{E}\left[(Y - \mathbb{E}\left[Y|\boldsymbol{X}_{2:d}\right])^2 | M_1' = 1 \right] \\ &= (1-p)\mathbb{E}\left[(Y - \mathbb{E}\left[Y|\boldsymbol{X}\right])^2 \right] + p\mathbb{E}\left[(Y - \mathbb{E}\left[Y|\boldsymbol{X}_{2:d}\right])^2 \right], \end{split}$$

where the last equality follows from the MAR assumption. Then we can apply the tower rule, conditioning on M_1 :

$$\begin{split} R' &= (1-p)\mathbb{E}\left[\mathbb{E}\left[(Y - \mathbb{E}\left[Y|\boldsymbol{X}\right])^2|M_1\right]\right] + p\mathbb{E}\left[\mathbb{E}\left[(Y - \mathbb{E}\left[Y|\boldsymbol{X}_{2:d}\right])^2|M_1\right]\right] \\ &= (1-p)^2\mathbb{E}\left[(Y - \mathbb{E}\left[Y|\boldsymbol{X}\right])^2|M_1 = 0\right] + p(1-p)\mathbb{E}\left[(Y - \mathbb{E}\left[Y|\boldsymbol{X}\right])^2|M_1 = 1\right] \\ &+ p(1-p)\mathbb{E}\left[(Y - \mathbb{E}\left[Y|\boldsymbol{X}_{2:d}\right])^2|M_1 = 0\right] + p^2\mathbb{E}\left[(Y - \mathbb{E}\left[Y|\boldsymbol{X}_{2:d}\right])^2|M_1 = 1\right] \\ &=: (1-p)^2A + p(1-p)(B+C) + p^2D. \end{split}$$

Then, we can modify the terms A, B, C, and D as follows:

$$A = \mathbb{E}\left[(Y - \mathbb{E}[Y|\boldsymbol{X}])^2 | M_1 = 0 \right]$$

$$= \mathbb{E}\left[(Y - \mathbb{E}[Y|\boldsymbol{X}, M_1] + \mathbb{E}[Y|\boldsymbol{X}, M_1] - \mathbb{E}[Y|\boldsymbol{X}])^2 | M_1 = 0 \right]$$

$$= \mathbb{E}\left[(Y - \mathbb{E}[Y|\boldsymbol{X}, M_1])^2 | M_1 = 0 \right] + \mathbb{E}\left[(\mathbb{E}[Y|\boldsymbol{X}, M_1] - \mathbb{E}[Y|\boldsymbol{X}])^2 | M_1 = 0 \right]$$

$$+ 2\mathbb{E}\left[(Y - \mathbb{E}[Y|\boldsymbol{X}, M_1]) (\mathbb{E}[Y|\boldsymbol{X}, M_1] - \mathbb{E}[Y|\boldsymbol{X}]) | M_1 = 0 \right]$$

$$= \mathbb{E}\left[(Y - \mathbb{E}[Y|\boldsymbol{X}, M_1])^2 | M_1 = 0 \right] + \psi_0(\boldsymbol{X}, \boldsymbol{X}),$$

since $\mathbb{E}[Y|X, M_1] - \mathbb{E}[Y|X]$ is constant when conditioning on X and M_1 , and $\mathbb{E}[(Y - \mathbb{E}[Y|X, M_1])|X, M_1] = 0$. Similarly, we can show that

$$B = \mathbb{E} \left[(Y - \mathbb{E} [Y | \mathbf{X}_{2:d}, M_1])^2 | M_1 = 1 \right] - \psi_1(\mathbf{X}, \mathbf{X}_{2:d}),$$

$$C = \mathbb{E} \left[(Y - \mathbb{E} [Y | \mathbf{X}, M_1])^2 | M_1 = 0 \right] + \psi_0(\mathbf{X}_{2:d}, \mathbf{X}),$$

$$D = \mathbb{E} \left[(Y - \mathbb{E} [Y | \mathbf{X}_{2:d}, M_1])^2 | M_1 = 1 \right] + \psi_1(\mathbf{X}_{2:d}, \mathbf{X}_{2:d}).$$

Putting it all together yields:

$$R' = (1 - p)\mathbb{E}\left[(Y - \mathbb{E}[Y|X, M_1])^2 | M_1 = 0 \right] + p\mathbb{E}\left[(Y - \mathbb{E}[Y|X_{2:d}, M_1])^2 | M_1 = 1 \right]$$

$$+ (1 - p)^2 \psi_0(X, X) + p^2 \psi_1(X_{2:d}, X_{2:d}) + p(1 - p)\psi_0(X_{2:d}, X) - p(1 - p)\psi_1(X, X_{2:d}).$$

Recognizing that the first two terms in the above expression are equal to R completes the proof.

Appendix C: Pseudocodes

C.1. Recursive partitioning for finitely adaptive linear regression

Algorithm 1: Iterative procedure for fintely adaptive regression Result: Partition $\mathcal{P} = \{\mathcal{M}_q, \ q \in [Q]\}$ and models $\{\boldsymbol{w}^q, \ q \in [Q]\}$.

initialization: $\mathcal{P} = \{\mathcal{M}_1 = \mathcal{M}\};$

for $\mathcal{M}_q \in \mathcal{P}$ do

$$j^{\star} \leftarrow \operatorname*{arg\,min}_{j, \boldsymbol{w}^{0}, \boldsymbol{w}^{1}} \sum_{i: \boldsymbol{m}_{i} \in \mathcal{M}_{q}^{j, 0}} \ell\left(y_{i}, \langle \boldsymbol{w}^{0}, \boldsymbol{x}_{i} \rangle_{\boldsymbol{m}_{i}}\right) + \sum_{i: \boldsymbol{m}_{i} \in \mathcal{M}_{q}^{j, 1}} \ell\left(y_{i}, \langle \boldsymbol{w}^{1}, \boldsymbol{x}_{i} \rangle_{\boldsymbol{m}_{i}}\right);$$

 ${\bf if}\ stopping\ criterion\ is\ not\ met\ {\bf then}$

split
$$\mathcal{M}_q$$
 along j^* : $\mathcal{P} \leftarrow (\mathcal{P} \setminus \{\mathcal{M}_q\}) \cup \{\mathcal{M}_q^{j^*,0}, \mathcal{M}_q^{j^*,1}\}$

end

end

C.2. Alternating optimization scheme for joint impute-then-regress

Algorithm 2: Heuristic iterative procedure for joint μ -impute-then-regress

Result: Vector of imputed values μ and predictive model f.

init

$$\mu_j \leftarrow \text{mean}(X_j | M_j = 0);$$

 $\sigma_j \leftarrow \text{std}(X_j) / \sqrt{n};$

repeat

 $f \leftarrow \text{best model to predict } Y \text{ given } \boldsymbol{X}^{\mu} ;$

repeat

$$\begin{array}{l} \textbf{for } j = 1, \dots, p \ \textbf{do} \\ & \epsilon_j \leftarrow \arg\min_{\epsilon \in \{-1, 0, 1\}} \, \operatorname{error} \left(Y, f \left(\boldsymbol{X}^{\mu + \epsilon \sigma_j \boldsymbol{e}_j} \right) \right); \\ & \mu_j \leftarrow \mu_j + \epsilon_j \sigma_j \end{array}$$

Appendix D: Technical lemmas for the proof of Theorem 3

LEMMA 1. For any $t \in \mathbb{Z}_+$, let $w_j^t(\boldsymbol{m})$ denote the order-t Taylor expansion of $w_j^*(\boldsymbol{m})$ at $\mathbb{E}[\boldsymbol{m}]$. Similarly, denote $f^t(\boldsymbol{x}, \boldsymbol{m}) = \sum_{j=1}^d w_j^t(\boldsymbol{m}) x_j (1 - m_j)$. Then,

$$|f^{\star}(\boldsymbol{x}, \boldsymbol{m}) - f^{t}(\boldsymbol{x}, \boldsymbol{m})| \leq \frac{2^{t+1}L}{(t+1)!} \|\boldsymbol{m} - \mathbb{E}[\boldsymbol{M}]\|^{t+1}.$$

Proof of Lemma 1 Let us consider the change of variable $\tilde{x}_j = x_j(1 - m_j)$ and the function (with a slight abuse of notations) $f^*(\tilde{\boldsymbol{x}}, \boldsymbol{m}) = \sum_j w_j^*(\boldsymbol{m})\tilde{x}_j$. If C is a uniform bound on the order-(t+1) derivatives of $f^*(\tilde{\boldsymbol{x}}, \cdot)$, then Taylor's theorem in multiple variables (Folland 2005, corollary 1) yields

$$|f^{\star}(\tilde{\boldsymbol{x}}, \boldsymbol{m}) - f^{t}(\tilde{\boldsymbol{x}}, \boldsymbol{m})| \leq \frac{C}{(t+1)!} \|\boldsymbol{m} - \mathbb{E}[\boldsymbol{M}]\|^{t+1}.$$

Accordingly, if we prove that order-t derivatives of $f^*(\tilde{x},\cdot)$ are bounded by 2^tL , then the result will follow. Consider a sequence of t indices, j_1, \ldots, j_t . Consider $j' \in \{1, \ldots, d\}$. Recall that

$$w_{j'}^{\star}(\mathbf{M}) = \sum_{\mathbf{m} \in \{0,1\}^d} w_{j',m}^{\star} \prod_{j=1}^d (1 - M_j - m_j + 2M_j m_j).$$

In particular, $w_{j'}^*(\mathbf{M})$ is linear in each coordinate M_j , all other coordinates being fixed. Hence, if the indices j_1, \ldots, j_t are not distinct,

$$\frac{\partial^t w_{j'}^{\star}}{\partial M_{j_1} \dots \partial M_{j_t}}(\boldsymbol{M}) = 0,$$

and

$$\frac{\partial^t f^\star}{\partial M_{j_1} \dots \partial M_{j_t}} (\tilde{\boldsymbol{X}}, \boldsymbol{M}) = 0.$$

as well. On the other hand, if the indices j_1, \ldots, j_t are distinct, we have

$$\frac{\partial^t w_{j'}^{\star}}{\partial M_{j_1} \dots \partial M_{j_t}}(\mathbf{M}) = \sum_{m \in \{0,1\}^d} w_{j',m}^{\star} \prod_{\tau=1}^t (2m_{j_{\tau}} - 1) \prod_{i \neq j_1, \dots, j_t} (1 - M_i - m_i + 2M_i m_i).$$

Observe that the product on the right-hand side is non-zero only for missingness patterns m that satisfy $M_i = m_i$ for all $i \neq j_1, \ldots, j_t$. So the sum over all missingness patterns m reduces to a sum over 2^t terms. Consequently,

$$\frac{\partial^{t} f^{\star}}{\partial M_{j_{1}} \dots \partial M_{j_{t}}} (\tilde{\boldsymbol{X}}, \boldsymbol{M}) = \sum_{j'=1}^{d} \sum_{m \in \{0,1\}^{d}} w_{j',m}^{\star} \tilde{X}_{j'} \prod_{\tau=1}^{t} (2m_{j_{\tau}} - 1) \prod_{i \neq j_{1}, \dots, j_{t}} (1 - M_{i} - m_{i} + 2M_{i}m_{i})$$

$$= \sum_{m \in \{0,1\}^{d}} \left(\sum_{j'=1}^{d} w_{j',m}^{\star} \tilde{X}_{j'} \right) \prod_{\tau=1}^{t} (2m_{j_{\tau}} - 1) \prod_{i \neq j_{1}, \dots, j_{t}} (1 - M_{i} - m_{i} + 2M_{i}m_{i}).$$

In the sum above, at most 2^t terms are non-zero. According to Assumption 1, $\left|\sum_{j'=1}^d w_{j',m}^{\star} \tilde{X}_{j'}\right| \leq L$. Furthermore, $\prod_{\tau=1}^t (2m_{j_\tau} - 1) \in \{-1,1\}$ so

$$\left| \frac{\partial^t f^*}{\partial M_{j_1} \dots \partial M_{j_t}} (\tilde{\boldsymbol{X}}, \boldsymbol{M}) \right| \leq 2^t L.$$

LEMMA 2. For any $t \in \mathbb{Z}_+$, let $w_j^t(\boldsymbol{m})$ denote the order-t Taylor expansion of $w_j^*(\boldsymbol{m})$ at $\mathbb{E}[\boldsymbol{m}]$. Similarly, denote $f^t(\boldsymbol{x}, \boldsymbol{m}) = \sum_{j=1}^d w_j^t(\boldsymbol{m}) x_j (1-m_j)$. Then,

$$\mathbb{E}\left[\left|f^{\star}(\boldsymbol{X},\boldsymbol{M})-f^{t}(\boldsymbol{X},\boldsymbol{M})\right|^{2}\right]=\mathcal{O}\left(\left(\frac{d}{(t+1)^{3}}\right)^{t+1}\right).$$

Proof of Lemma 2 By Lemma 1, we have

$$\mathbb{E}\left[\left|f^{\star}(\boldsymbol{X},\boldsymbol{M})-f^{t}(\boldsymbol{X},\boldsymbol{M})\right|^{2}\right] \leq \frac{4^{t+1}L^{2}}{\left(\left(t+1\right)!\right)^{2}}\mathbb{E}\left[\left\|\boldsymbol{M}-\mathbb{E}[\boldsymbol{M}]\right\|^{2(t+1)}\right].$$

Since $\|\boldsymbol{M} - \mathbb{E}[\boldsymbol{M}]\|^2 = \sum_{j=1}^d (M_j - \mathbb{E}[M_j])^2 \le d/4$, $\mathbb{E}\left[\|\boldsymbol{M} - \mathbb{E}[\boldsymbol{M}]\|^{2(t+1)}\right] \le (d/4)^{t+1}$ and we obtain

$$\mathbb{E}\left[\left|f^{\star}(\boldsymbol{X},\boldsymbol{M})-f^{t}(\boldsymbol{X},\boldsymbol{M})\right|^{2}\right] \leq \frac{d^{t+1}L^{2}}{\left((t+1)!\right)^{2}}.$$

Using Stirling's approximation $(t+1)! \sim \sqrt{2\pi(t+1)}(\frac{t+1}{e})^{t+1}$ yields the result.

Appendix E: Description of the data and evaluation methodology

In this section, we describe the datasets we used in our numerical experiments, as well as various implementation details. In line with other works in the literature, we conduct some of our experiments on synthetic data, where we have full control over the design matrix X, the missingness pattern M, and the signal Y. We also contrast the results obtained on these synthetic instances with real world instances from the UCI Machine Learning Repository and the RDatasets Repository³.

E.1. Synthetic data generation

As in Le Morvan et al. (2020, section 7), we generate a multivariate vector \boldsymbol{X} from a multivariate Gaussian with mean 0 and covariance matrix $\boldsymbol{\Sigma} := \boldsymbol{B}\boldsymbol{B}^\top + \epsilon \mathbb{I}$ where $\boldsymbol{B} \in \mathbb{R}^{d \times r}$ with i.i.d. standard Gaussian entries and $\epsilon > 0$ is chosen small enough so that $\boldsymbol{\Sigma} \succ \boldsymbol{0}$. We fix d = 10 and r = 5 in our experiments. We generate a n observations, $n \in \{20, 40, \dots, 1000\}$, for the training data and 5,000 observations for the test data.

We then generate signals $Y = f(X) + \varepsilon$, where $f(\cdot)$ is a predefined function and ε is a centered normal random noise whose variance is calibrated to achieve a target signal-to-noise ratio SNR. We choose SNR = 2 in our experiments. We use functions $f(\cdot)$ of the following forms:

- Linear model: $f(x) = b + w^{\top}x$ where $b \sim \mathcal{N}(0,1)$ and $w_j \sim \mathcal{U}([-1,1])$.
- Neural Network (NN) model: f(x) corresponds to the output function of a 2-layer neural network with 10 hidden nodes, ReLU activation functions, and random weights and intercept for each node.

We compute f(x) using a random subset of k out of the d features only, with k=5.

Finally, for a given fraction of missing entries p, we generate missing entries according to mechanisms

- Missing Completely At Random (MCAR): For each observation and for each feature $j \in \{1, ..., d\}$, we sample $M_j \sim Bern(p)$ independently (for each feature and each observation).
- Not Missing At Random (NMAR) Censoring: We set $M_j = 1$ whenever the value of X_j is above the (1-p)th percentile.

https://archive.ics.uci.edu and https://github.com/vincentarelbundock/Rdatasets

For the fraction of missing entries, we consider the different values $p \in \{0.1, 0.2, \dots, 0.8\}$.

With this methodology, we generate a total of 50 training sets, with 2 categories of signal Y, 2 missingness mechanisms, and 8 proportion of missing entries, i.e., 1,600 different instances.

We measure the predictive power of a method in terms of average out-of-sample \mathbb{R}^2 . We use \mathbb{R}^2 , which is a scaled version of the mean squared error, to allow for a fair comparison and aggregation of the results across datasets and generative models.

E.2. Real-world design matrix

In addition to synthetic data, we also assemble a corpus of 63 publicly available datasets with missing data, from the UCI Machine Learning Repository and the RDatasets Repository. Tables 5, 6, and 7 present summary statistics for the datasets with only categorical features missing, only continuous features missing, and both categorical and continuous features missing respectively. We use the datasets presented in Tables 5 and 7 in Section 3.2, to empirically validate that, for categorical features, missingness should be encoded as a category instead of using mode imputation. Then, we use the datasets from Tables 6 and 7 in Section 3.3, to compare the performance of different impute-then-regress strategies and our adaptive regression models.

For these datasets, we consider two categories of signal Y, real-world and synthetic signals.

Dataset	$\mid n \mid$	#features	#missing cont.	#missing cat.	$ \mathcal{M} $	d	Y
Ecdat-Males	4360	37	0	4	2	38	cont.
mushroom	8124	116	0	4	2	117	bin.
post-operative-patient	90	23	0	4	2	24	bin.
breast-cancer	286	41	0	7	3	43	bin.
heart-disease-cleveland	303	28	0	8	3	30	bin.
COUNT-loomis	384	9	0	9	4	12	cont.
Zelig-coalition2	314	24	0	14	2	25	NA
shuttle-landing-control	15	16	0	16	6	21	bin.
congressional-voting-records	435	32	0	32	60	48	bin.
lung-cancer	32	157	0	33	3	159	bin.
soybean-large	307	98	0	98	8	132	bin.

Table 5 Description of the 11 datasets in our library where the features affected by missingness are categorical features only. n denotes the number of observations. The columns '#features', '#missing cont.', and '#missing cat.' report the total number of features, the number of continuous features affected by missingness, and the number of categorical features affected by missingness, respectively. $|\mathcal{M}|$ correspond to the number of unique missingness patterns $m \in \{0,1\}^d$ observed, where d is the total number of features after one-hot-encoding of the categorical features. The final column Y indicates whether the dependent variable is binary or continuous (if available).

Dataset	n	$\# {\rm features}$	# missing cont.	$\# {\rm missing} \ {\rm cat}.$	$ \mathcal{M} $	d	Y
auto-mpg	398	13	1	0	2	13	cont.
breast-cancer-wisconsin-original	699	9	1	0	2	9	bin.
breast-cancer-wisconsin-prognostic	198	32	1	0	2	32	bin.
dermatology	366	130	1	0	2	130	cont.
ggplot2-movies	58788	34	1	0	2	34	NA
indian-liver-patient	583	11	1	0	2	11	bin.
rpart-car.test.frame	60	81	1	0	2	81	bin.
Ecdat-MCAS	180	13	2	0	3	13	cont.
MASS-Cars93	93	64	2	0	3	64	cont.
car-Davis	200	6	2	0	4	6	NA
car-Freedman	110	4	2	0	2	4	NA
car-Hartnagel	37	8	2	0	2	8	NA
datasets-airquality	153	4	2	0	4	4	NA
mlmRev-Gcsemv	1905	77	2	0	3	77	NA
MASS-Pima.tr2	300	7	3	0	6	7	bin.
Ecdat-RetSchool	3078	37	4	0	8	37	cont.
arrhythmia	452	391	5	0	7	391	cont.
boot-neuro	469	6	5	0	9	6	NA
reshape2-french_fries	696	9	5	0	4	9	NA
survival-mgus	241	15	5	0	11	15	bin.
sem-Tests	32	6	6	0	8	6	NA
robustbase-ambientNOxCH	366	13	13	0	45	13	NA

Table 6 Description of the 22 datasets in our library where the features affected by missingness are numerical features only. n denotes the number of observations. The columns '#features', '#missing cont.', and '#missing cat.' report the total number of features, the number of continuous features affected by missingness, and the number of categorical features affected by missingness, respectively. $|\mathcal{M}|$ correspond to the number of unique missingness patterns $m \in \{0,1\}^d$ observed, where d is the total number of features after one-hot-encoding of the categorical features. The final column Y indicates whether the dependent variable is binary or continuous (if available).

Dataset	n	#features	#missing cont.	#missing cat.	$ \mathcal{M} $	d	Y
pscl-politicalInformation	1800	1440	1	1431	3	1441	bin.
car-SLID	7425	8	2	3	8	9	NA
rpart-stagec	146	15	2	3	4	16	NA
Ecdat-Schooling	3010	51	2	8	9	53	cont.
mammographic-mass	961	15	2	13	9	18	bin.
cluster-plantTraits	136	68	2	37	16	85	NA
mlmRev-star	24613	122	2	72	19	128	cont.
car-Chile	2532	14	3	3	7	15	bin.
heart-disease-hungarian	294	25	3	17	16	31	bin.
heart-disease-switzerland	123	26	3	18	12	32	bin.
ggplot2- $msleep$	83	35	3	29	15	37	NA
survival-cancer	228	13	4	4	8	14	cont.
heart-disease-va	200	25	4	13	18	30	bin.
MASS-survey	237	24	4	19	8	29	NA
hepatitis	155	32	5	20	21	42	bin.
automobile	205	69	6	2	7	70	cont.
echocardiogram	132	8	6	2	13	9	bin.
thyroid-disease-allbp	2800	52	6	46	25	54	bin.
thyroid-disease-allhyper	2800	52	6	46	25	54	bin.
thyroid-disease-allhypo	2800	52	6	46	25	54	bin.
thyroid-disease-allrep	2800	52	6	46	25	54	bin.
thyroid-disease-dis	2800	52	6	46	25	54	bin.
thyroid-disease-sick	2800	52	6	46	25	54	bin.
survival-pbc	418	27	7	17	8	32	bin.
thyroid-disease-sick-euthyroid	3163	43	7	36	23	44	bin.
horse-colic	300	60	7	52	171	73	bin.
plyr-baseball	21699	296	9	14	18	297	NA
communities-and-crime	1994	126	22	3	4	127	cont.
communities-and-crime-2	2215	129	22	3	4	130	cont.
wiki4he	913	73	44	24	236	78	cont.

Table 7 Description of the 30 datasets in our library where the features affected by missingness are numerical features only. n denotes the number of observations. The columns '#features', '#missing cont.', and '#missing cat.' report the total number of features, the number of continuous features affected by missingness, and the number of categorical features affected by missingness, respectively. $|\mathcal{M}|$ correspond to the number of unique missingness patterns $m \in \{0,1\}^d$ observed, where d is the total number of features after one-hot-encoding of the categorical features. The final column Y indicates whether the dependent variable is binary or continuous (if available).

E.2.1. Real signal Y 46 out of the 63 datasets had an identified target variable Y, which could be continuous or binary. If Y is categorical with more than 1 category, we considered the binary one-vs-all classification task using the first (alphabetical order) category. For regression (resp. classification) tasks, we use the mean squared error (resp. logistic log-likelihood) as the training loss and measure predictive power in terms of R^2 (resp. $2 \times AUC - 1$). Again, we choose this measure over mean square error (resp. accuracy or AUC) because it is normalized between 0 and 1, and can be more safely compared and aggregated across datasets.

E.2.2. Synthetic signal Y To generate synthetic signals Y, we use the same three generative models as with synthetic data in Section E.1. However, this requires knowledge of the fully observed input matrix, while we only have access to observations with missing entries, $(o(\boldsymbol{x}^{(i)}, \boldsymbol{m}^{(i)}), \boldsymbol{m}^{(i)}), i = 1, ..., n$. Therefore, we first generate a fully observed version of the data by performing missing data imputation using the R package missForest (Stekhoven and Bühlmann 2012), obtaining a new dataset $\{(\boldsymbol{x}_{\text{full}}^{(i)}, \boldsymbol{m}^{(i)})\}_{i \in [n]}$. We use this dataset to generate synthetic signals Y, using the three types of signals described in Section E.1: linear, tree, and neural network.

Regarding the relationship between the missingness pattern M and the signal Y, we consider three mechanisms:

- MAR: In this setting, we pass $k = \min(10, d)$ coordinates of $\boldsymbol{x}_{\text{full}}$ as input to the function $f(\cdot)$. Out of these k features, we explicitly control $k_{missing} \in \{0, \dots, k\}$, the number of features contributing to the signal that are affected by missingness. Hence, in this setting, the resulting response Y depends directly on the covariates \boldsymbol{X} but not on the missingness pattern \boldsymbol{M} . However, we do not control the correlation between \boldsymbol{X} and \boldsymbol{M} for two reasons: First, they both come from a real-world dataset which might not satisfy the MAR assumption. Second, as previously observed (Remark 1), imputation does induce some correlation between the imputed dataset \boldsymbol{X}_{full} and \boldsymbol{M} .
- NMAR: In the second setting, in addition to k = 10 coordinates of $\boldsymbol{x}_{\text{full}}$, we also pass $k_{missing}$ coordinates of \boldsymbol{m} , so that Y is now a function of both \boldsymbol{X} and \boldsymbol{M} .
- Adversarially Missing (AM): The third setting generates Y in the same way as the MAR setting. After Y is generated, however, we reallocate the missingness patterns across observations so as to ensure the data is NMAR. Formally, we consider the observations $(o(\boldsymbol{x}_{\text{full}}^{(i)}, \boldsymbol{m}^{(\sigma_i)}), \boldsymbol{m}^{(\sigma_i)}, y^{(\sigma_i)}), i \in [n]$, where σ is the permutation maximizing the total sum of missing values $\sum_{i=1}^{n} \boldsymbol{x}_{\text{full}}^{(i)^{\top}} \boldsymbol{m}^{(\sigma_i)}$.

For each real-world dataset, this methodology generates up to $3 \times 3 \times 11 = 66$ different instances.

All together, we obtain four experimental settings, with both synthetic and real signals Y. They differ in the relationships between the missingness pattern M, the design matrix X and the signal Y as summarized on Figure 9.

E.3. Evaluation pipeline

In our numerical experiments, we compare a series of approaches, namely

• Regression on the features that are never missing only (complete-feature regression).

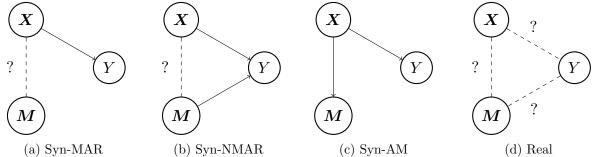


Figure 9 Graphical representation of the 4 experimental designs implemented in our benchmark simulations with real-world design matrix X. Solid (resp. dashed) lines correspond to correlations explicitly (resp. not explicitly) controlled in our experiments.

- Impute-then-regress methods where the imputation step is performed either via mean imputation or using the chained equation method mice (van Buuren and Groothuis-Oudshoorn 2010). We implement these two approaches with a linear, tree, or random forest model for the downstream predictive model. We treat the type of model as an hyper-parameter. We used the default parameter values for number of imputations and number of iterations in mice.
- Three variants of the adaptive linear regression framework from Section 4: Static coefficients with affine intercept, affine coefficients and intercept, finitely adaptive.
- The joint impute-then-regress heuristic presented in Section 5. Again, we consider three downstream predictive models: linear, tree, random forest.

For adaptive linear regression models with affine intercept or affine coefficients, the hyper-parameters are the Lasso penalty λ , the amount of ridge regularization α (ElasticNet), and the additional lasso penalty for the adaptive coefficients. For the finitely adaptive linear regression model, the only hyper-parameter is the maximum depth of the tree. The other methods can all be applied with linear, tree-based, or random forest predictors. For linear predictors, the hyper-parameters are the Lasso penalty λ and the amount of ridge regularization α (ElasticNet). For tree predictors, the hyper-parameter is the maximum depth. For the random forest predictors, the hyper-parameters are the maximum depth of each tree and the number of trees in the forest.

All hyper-parameters are cross-validated using a 5-fold cross-validation procedure on the training set.

We report out-of-sample predictive power on the test set. For synthetic data, the test set consists of 5,000 observations. For real data, we hold out 30% of the observations as a test set.

All experiments are replicated 10 times, with different (random) split into training/test sets between replications.

Appendix F: Discussion: Implementation of impute-then-regress pipelines in practice

As discussed in Section 3.1, to achieve the best achievable predictive power, Theorem 1 requires the imputation rule to be the same on the training set (on which the downstream predictive model is then trained) as on the test set. However, many imputation models (especially the best performing ones) do not impute

Table 8 Regression output for predicting the out-of-accuracy (R^2 or AUC) based on the implementation of the impute-then-regress method. We include dataset and $k_{misssing}$ fixed effects. We report regression coefficient values (and clustered standard errors).

Signal Y	Missingness	V1 vs. V2 coeff.	V3 vs. V2 coeff.	Adjusted \mathbb{R}^2
Synthetic - Linear	MAR	0.0051 (0.0042)	-0.0029 (0.0032)	0.4947
	NMAR	-0.0021 (0.0027)	-0.0037 (0.0028)	0.4760
	AM	0.0004 (0.0025)	-0.0003 (0.0008)	0.5704
Synthetic - NN	MAR	-0.0047 (0.0054)	-0.0022 (0.0014)	0.1106
	NMAR	0.0082 (0.0044)*	-0.0045 (0.0023)*	0.2932
	AM	0.0051 (0.0035)	-0.0012 (0.0009)	0.4602
Real	Real	0.0008 (0.0038)	0.0006 (0.0010)	0.7893

Controls: Dataset, $k_{missing}$ (if available); p-value: *:< 0.1, **:< 0.01

missing values as a simple function of the observed features but rely on an iterative process where, at each iteration, current imputed values are used to train a new imputation model and then updated. Consequently, in practice, we cannot guarantee that the exact same imputation rule is used in training and testing.

We consider three implementations of impute-then-regress:

- (V1) In the first variant, we simultaneously impute the train and test set, before training the model.
- (V2) Secondly, we impute the training set alone, and then impute the test set with the *imputed* training data.

(V3) As a third option, we impute the training set alone and then the test set with the *original* training set. Intuitively, (V1) should lead to the most consistent imputation across the training and test set but is not practical for predictive models that are meant to be used in production. Indeed, the behavior of the model on the test set should mimic its behavior on future observations, which, by definition, are unavailable (hence should not be used) at any stage of the calibration process. (V2) is the variant we compared mean-imputation against in Section 3.3. We intuit that (V3) will be less powerful than (V2) because the rules learned for imputing the test set might differ from the ones used for the training set.

We conduct a regression analysis (Table 8), to assess the relative benefit of using (V1) and (V3) over (V2). Overall, we observe that no statistically significant difference between the three variants. Henceforth, we recommend in practice to use (V2) since it mimics more closely the production pipeline and the theoretical requirements from Theorem 1.