Missing Data Imputation using Optimal Transport

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Abstract

Missing data is a crucial issue when applying machine learning algorithms to real-world datasets. Starting from the simple assumption that two batches extracted randomly from the same dataset should share the same distribution, we leverage optimal transport distances to quantify that criterion and turn it into a loss function to impute missing data values. We propose practical methods to minimize these losses using end-to-end learning, that can exploit or not parametric assumptions on the underlying distributions of values. We evaluate our methods on datasets from the UCI repository, in MCAR, MAR and MNAR settings. These experiments show that OT-based methods match or out-perform state-of-the-art imputation methods, even for high percentages of missing values.

1. Introduction

Data collection is usually a messy process, resulting in datasets that have many missing values. This has been an issue for as long as data scientists have prepared, curated and obtained data, and is all the more inevitable given the vast amounts of data currently collected. The literature on the subject is therefore abundant (Little & Rubin, 2019; van Buuren, 2018): a recent survey indicates that there are more than 150 implementations available to handle missing data (Mayer et al., 2019). These methods differ on the objectives of their analysis (estimation of parameters and their variance, matrix completion, prediction), the nature of the variables considered (categorical, mixed, etc), the assumptions about the data, and the missing data mechanisms. Imputation methods, which consist in filling missing entries with plausible values are very appealing as they allow to both get a guess for the missing entries as well as to perform (with care) downstream machine learning methods on the completed data. Efficient methods include, among others, methods based on low-rank assumptions (Hastie et al., 2015), iterative random forests (Stekhoven & Bühlmann, 2011) and imputation using a variational autoencoder (Mattei & Frellsen, 2019). A desirable property for imputation methods is that they should preserve the joint and marginal distributions of the data. Non-parametric Bayesian strategies (Murray & Reiter, 2016) or recent approaches based on generative adversarial networks (Yoon et al., 2018) are attempts in this direction. However, they are quite cumbersome.

We argue in this work that the optimal transport (OT) toolbox constitutes a natural, sound and straightforward alternative. Indeed, optimal transport provides geometrically meaningful distances to compare discrete distributions in various spaces (namely data). Furthermore, thanks to recent computational advances grounded on regularization (Cuturi, 2013), OT-based divergences can be computed in a scalable and differentiable way (Peyré et al., 2019). Those advances have allowed to successfully use OT as a loss function in many applications, including among others multi-label classification (Frogner et al., 2015), inference of pathways (Schiebinger et al., 2019) and generative modeling (Arjovsky et al., 2017; Genevay et al., 2018; Salimans et al., 2018). Considering the similarities between generative modeling and missing data imputation, it is therefore quite natural to use OT as a loss for the latter.

Contributions. This paper presents two main contributions. First, we leverage OT to define a loss function for missing value imputation. This loss function is the mathematical translation of the simple intuition that two random batches from the same dataset should follow the same distribution. Next, we provide algorithms for imputing missing values according to that loss. Two types of algorithms are presented, the first (i) being non-parametric, and the second (ii) defining a class of parametric models. The non-parametric algorithm (i) enjoys the most degrees of freedom, and can therefore output imputations which respect the global shape of the data while taking into account its local features. The parametric algorithm (ii) is trained in a round robin fashion similar to iterative conditional imputation techniques, as implemented for instance in the mice pipeline (van Buuren & Groothuis-Oudshoorn, 2019).
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2011). Compared to the non-parametric method, this algorithm allows to perform out-of-sample imputation. This creates a very flexible framework which can be combined with many imputing strategies, including imputation with Multi-Layer Perceptrons. Finally, these methods are showcased in extensive experiments on a variety of datasets and for different missing values proportions and missing values mechanisms, including the difficult case of informative missing entries. Our code is available at https://github.com/BorisMuzellec/MissingDataOT.

Notations. Let $\Omega = (\omega_{ij})_{ij} \in \{0, 1\}^{n \times d}$ be a binary mask encoding observed entries, i.e. $\omega_{ij} = 1$ (resp. 0) iff the entry $(i, j)$ is observed (resp. missing). We observe the following incomplete data matrix:

$$X = X^{(obs)} \odot \Omega + \mathbf{X}^{(imp)} \odot (\mathbf{I}_{n \times d} - \Omega),$$

where $X^{(obs)} \in \mathbb{R}^{n \times d}$ contains the observed entries, $\odot$ is the elementwise product and $\mathbf{I}_{n \times d}$ is an $n \times d$ matrix filled with ones. Given the data matrix $X$, our goal is to construct an estimate $\hat{X}$ filling the missing entries of $X$, which can be written as

$$\hat{X} = X^{(obs)} \odot \Omega + \hat{X}^{(imp)} \odot (\mathbf{I}_{n \times d} - \Omega),$$

where $\hat{X}^{(imp)} \in \mathbb{R}^{n \times d}$ contains the imputed values. Let $x_i$ denote the $i$-th row of the data set $X$, such that $X = \{(x_i^T)_{1 \leq i \leq n}\}$. Similarly, $x_j$ denotes the $j$-th column (variable) of the data set $X$, such that $X = \{x_1 \ldots x_d\}$. We denote by $X_{i:,j}$ the dataset $X$ in which the $j$-th variable has been removed. For $K \subset \{1, \ldots, n\}$ a set of $m$ indices, we denote by $X_K = (x_k)_{k \in K}$ the corresponding batch, and by $\mu_m(X_K)$ the empirical measure associated to $X_K$, i.e.

$$\mu_m(X_K) := \frac{1}{m} \sum_{k \in K} \delta_{x_k}.$$ 

$$\Delta_n \overset{\text{def}}{=} \{\mathbf{a} \in \mathbb{R}_+^n : \sum_{i=1}^n a_i = 1\}$$

is the simplex in dimension $n$.

2. Background

Missing Data. Rubin (1976) defined a widely used - yet controversial (Seaman et al., 2013) - nomenclature for missing values mechanisms. This nomenclature comprises three cases: missing completely at random (MCAR), missing at random (MAR), and missing not at random (MNAR). In MCAR, the missingness is independent of the data, whereas in MAR, the probability of being missing depends only on observed values. A subsequent part of the literature, with notable exceptions (Kim & Ying, 2018; Mohan & Pearl, 2019), only consider these ‘simple’ mechanisms and struggles for the harder yet prevalent MNAR case. MNAR values lead to important biases in the data, as the probability of missingness then depends on the unobserved values. On the other hand, MCAR and MAR are ‘ignorable’ mechanisms in the sense that they do not make it necessary to model explicitly the distribution of missing values when maximizing the observed likelihood.

The naive workaround which consists in deleting observations with missing entries is not an alternative in high dimension. Indeed, as exemplified in Zhu et al. (2019), assume that $X$ is an $n \times d$ data matrix in which each entry is missing independently with probability 0.01. When $d = 5$, this would result in around 95% of the individuals (rows) being retained, but for $d = 300$, only around 5% of rows have no missing entries. Hence, providing plausible imputations for missing values quickly becomes necessary. Classical imputation methods impute according to a joint distribution which is either explicit, or implicitly defined through a set of conditional distributions. As an example, explicit joint modeling methods include imputation models that assume a Gaussian distribution for the data, whose parameters are estimated using EM algorithms (Dempster et al., 1977). Missing values are then imputed by drawing from their predictive distribution. A second instance of such joint modeling methods are imputations assuming low-rank structure (Josse et al., 2016). The conditional modeling approach (van Buuren, 2018), also known as ‘sequential imputation’ or ‘imputation using chained equations’ (ice) consists in specifying one model for each variable. It predicts the missing values of each variable using the other variables as explanatory, and cycles through the variables iterating this procedure to update the imputations until predictions stabilize.

Non-parametric methods like $k$-nearest neighbors imputation (Troyanskaya et al., 2001) or random forest imputation (Stekhoven & Bühlmann, 2011) have also been developed and account for the local geometry of the data. The herein proposed methods lie at the intersection of global and local approaches and are derived in a non-parametric and parametric version.

Wasserstein distances, entropic regularization and Sinkhorn divergences. Let $\alpha = \sum_{i=1}^n a_i \delta_{x_i}$, $\beta = \sum_{i'=1}^{n'} b_i \delta_{y_{i'}}$ be two discrete distributions, described by their supports $\{(x_i)_{i=1}^n\} \in \mathbb{R}^{n \times p}$ and $\{(y_{i'})_{i'=1}^{n'}\} \in \mathbb{R}^{n' \times p}$ and weight vectors $\mathbf{a} \in \Delta_n$ and $\mathbf{b} \in \Delta_{n'}$. The Wasserstein distance between $\alpha$ and $\beta$ is defined as

$$W_2^2(\alpha, \beta) \overset{\text{def}}{=} \min_{\mathbf{P} \in U(\mathbf{a}, \mathbf{b})} \langle \mathbf{P}, \mathbf{M} \rangle,$$

where $U(\mathbf{a}, \mathbf{b}) \overset{\text{def}}{=} \{\mathbf{P} \in \mathbb{R}^{n \times n'} : \mathbf{P} \mathbb{1}_n = \mathbf{a}, \mathbf{P}^T \mathbb{1}_n = \mathbf{b}\}$ is the set of transportation plans, and $\mathbf{M} = (\|x_i - y_{i'}\|^2)_{ij} \in \mathbb{R}^{n \times n'}$ is the matrix of pairwise squared distances between the supports. $W_2$ is not differentiable and requires solving a costly linear program via network simplex methods (Peyré et al., 2019, §3). Entropic regularization alleviates both
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issues: consider
\[
\text{OT}_\varepsilon(\alpha, \beta) \overset{\text{def}}{=} \min_{P \in U(\alpha, \beta)} \langle P, M \rangle + \varepsilon h(P),
\]
where \(\varepsilon > 0\) and \(h(P) \overset{\text{def}}{=} \sum_{ij} p_{ij} \log p_{ij}\) is the negative entropy. Then, \(\text{OT}_\varepsilon(\alpha, \beta)\) is differentiable and can be solved using Sinkhorn iterations (Cuturi, 2013). However, due to the entropy term, \(\text{OT}_\varepsilon\) is no longer positive. This issue is solved through debiasing, by subtracting auto-correlation terms. Let
\[
S_\varepsilon(\alpha, \beta) \overset{\text{def}}{=} \text{OT}_\varepsilon(\alpha, \beta) - \frac{1}{2}(\text{OT}_\varepsilon(\alpha, \alpha) + \text{OT}_\varepsilon(\beta, \beta)).
\]
Eq. (3) defines the Sinkhorn divergences (Genevay et al., 2018), which are positive, convex, and can be computed with little additional cost compared to entropic OT (Feydy et al., 2019).

**OT gradient-based methods.** Not only are the OT metrics described above good measures of distribution closeness, they are also well-adapted to gradient-based imputation methods. Indeed, let \(X_K, X_L\) be two batches drawn from \(X\). Then, gradient updates for \(\text{OT}_\varepsilon(\mu_m(X_K), \mu_m(X_L)), \varepsilon \geq 0\) w.r.t a point \(x_{k_l}\) in \(X_K\) correspond to taking steps along the so-called barycentric transport map. Indeed, with (half) quadratic costs, it holds (Cuturi & Doucet, 2014, §4.3) that:
\[
\nabla_{x_k} \text{OT}_\varepsilon(\mu_m(X_K), \mu_m(X_L)) = \sum_{l} P_{k_l}^{*}(x_k: - x_L),
\]
where \(P^{*}\) is the optimal (regularized) transport plan. Therefore, a gradient based-update is of the form
\[
x_{k_l} \leftarrow (1 - t)x_{k_l} + t \sum_{l} P_{k_l}^{*} x_L.l.
\]
In a missing value imputation context, Eq. (4) thus corresponds to updating values to make them closer to the target points given by transportation plans. Building on this fact, OT gradient-based imputation methods are proposed in the next section.

3. Imputing Missing Values using OT

Let \(X_K\) and \(X_L\) be two batches respectively extracted from the complete rows and the incomplete ones in \(X\), such that only the batch \(X_L\) contains missing values. Then, a good imputation should preserve the distribution from the complete batch, meaning that both batches \(X_K\) and \(X_L\) should be close to each other in terms of distributions. The OT-based metrics described in Section 2 provide natural criteria to catch this distributional proximity in this one-sided incomplete batch setting. However, as observed in Section 2, in high dimension or with a high proportion of missing values, it is unlikely or even impossible to obtain batches from \(X\) with no missing values. Nonetheless, a good imputation method should still ensure that the distributions of any two i.i.d. incomplete batches \(X_K\) and \(X_L\), both containing missing values, should be close. This criterion is weaker than the one above with one-sided missing data, and will be considered from now on.

**Direct imputation.** Algorithm 1 aims at imputing missing values for quantitative variables: after initializing missing values of any variable with the mean of its observed entries plus a small amount of noise (to preserve the marginals and to facilitate the optimization), batches are sequentially sampled and the Sinkhorn divergence between batches is minimized with respect to the imputed values. Among the OT metrics described in Section 2, the use of Sinkhorn divergences is motivated by the fact that they are a differentiable and tractable proxy for Wasserstein distances. The imputation update is performed using RMSprop (Tieleman & Hinton, 2012).

**Algorithm 1 Batch Sinkhorn Imputation**

**Input:** \(X \in \mathbb{R}^{n \times d} \cup \{\text{NA}\}^{n \times d}, \Omega \in \{0, 1\}^{n \times d}, \alpha, \eta, \varepsilon > 0, n \geq m > 0\).

**Initialization:** for \(j = 1, \ldots, d\),
- for i.s.t. \(\omega_{ij} = 0\), \(\hat{x}_{ij} \leftarrow \frac{x_{ij}^{\text{obs}}}{\omega_{ij}^{\text{obs}}} + \varepsilon_{ij}\), with \(\varepsilon_{ij} \sim \mathcal{N}(0, \eta)\) and \(x_{ij}^{\text{obs}}\) corresponds to the mean of the observed entries in the \(j\)-th variable (missing entries)
- for i.s.t. \(\omega_{ij} = 1\), \(\hat{x}_{ij} \leftarrow x_{ij}\) (observed entries)

for \(t = 1, 2, \ldots, \text{max}\) do
Sample two sets \(K\) and \(L\) of \(m\) indices
\[
\mathcal{L}(\hat{X}_K, \hat{X}_L) \leftarrow S_{\varepsilon}(\mu_m(\hat{X}_K), \mu_m(\hat{X}_L))
\]
\[
\hat{X}_{K \cup L}^{\text{imp}} \leftarrow \hat{X}_{K \cup L} - \alpha \text{RMSprop}(\nabla_{\hat{X}_{K \cup L}^{\text{imp}}} \mathcal{L})
\]
end for

**Output:** \(\hat{X}\)

**OT as a loss for missing data imputation.** Taking a step back, one can see that Algorithm 1 essentially uses Sinkhorn divergences between batches as a loss function to impute values for a model in which “one parameter equals one imputed value”. Formally, for a fixed batch size \(m\), this loss is defined as
\[
\mathcal{L}_m(X) \overset{\text{def}}{=} \sum_{K: 0 \leq k_1 < \ldots < k_m \leq n} S_{\varepsilon}(\mu_m(X_K), \mu_m(X_L)).
\]
Eq. (5) corresponds to the “autocorrelation” counterpart of the minibatch Wasserstein distances described in Fatras et al. (2019); Salimans et al. (2018).

Although Algorithm 1 is straightforward, a downside is that it cannot directly generate imputations for out-of-sample
data points with missing values. Hence, a natural extension is to use the loss defined in Eq. (5) to fit parametric imputation models, provided they are differentiable with respect to their parameters. At a high level, this method is described by Algorithm 2. Algorithm 2 takes as an input an imputer model with a parameter $\Theta$ such that $\text{Imputer}(X, \Omega, \Theta)$ returns imputations for the missing values in $X$. This imputer has to be differentiable w.r.t. its parameter $\Theta$, so that the batch Sinkhorn loss $L$ can be back-propagated through $X$ to perform gradient-based updates of $\Theta$. Algorithm 2 does not only return the completed data matrix $\hat{X}$, but also the trained parameter $\hat{\Theta}$, which can then be re-used to impute missing values in out-of-sample data.

Round robin imputation. A remaining unaddressed point in Algorithm 2 is how to perform the “$\hat{X} \leftarrow \text{Imputer}(\hat{X}', \Omega, \hat{\Theta})$” step in the presence of missing values. A classical method is to perform imputations over variables in a round robin fashion, i.e. iteratively predicting missing coordinates using other coordinates as features in a cyclical manner. This corresponds to the case where the imputer parameter $\Theta$ is separable with respect to each variable ($x_{ij}$), i.e. $\Theta$ consists in $d$ sets of parameters $(\theta_j)_{1 \leq j \leq d}$ where each $\theta_j$ refers to the parameters used to predict the $j$-th variable. The $j$-th variable is iteratively imputed using the $d-1$ remaining variables, according to the chosen model with parameter $\theta_j$: $\theta_j$ is first fitted (using e.g. regression or Bayesian methods), then the $j$-th variable is imputed. The algorithm then moves to the next variable $j+1$, in a cyclical manner. This round robin method is implemented for instance in R’s mice package (van Buuren & Groothuis-Oudshoorn, 2011) or in the IterativeImputer method of the scikit-learn (Pedregosa et al., 2011) package. Making this round robin imputation explicit in the step “$\hat{X} \leftarrow \text{Imputer}(\hat{X}', \Omega, \hat{\Theta})$” of Algorithm 2 leads to Algorithm 3.

Algorithm 3 Round Robin Sinkhorn Imputation

```
Input: $X \in \mathbb{R}^{n \times d}$, $\Omega \in \{0, 1\}^{n \times d}$, Imputer(·, ·, ·), $\Theta_0$, $\epsilon > 0$, $n \geq m > 0$,
$X^0 \leftarrow$ same initialization as in Algorithm 1
for $t = 1, 2, ..., t_{\text{max}}$ do
  for $j = 1, 2, ..., d$ do
    for $k = 1, 2, ..., K$ do
      $\hat{X}_{ij} \leftarrow \text{Imputer}(\hat{X}_{i,j}', \Omega_j, \hat{\theta}_j)$
      Sample two sets $K$ and $L$ of $m$ indices
      $L \leftarrow S_{\epsilon}(\mu_m(X_K), \mu_m(X_L))$
      $\nabla_{\theta_j} L \leftarrow \text{AutoDiff}(L)$
      $\hat{\theta}_j \leftarrow \hat{\theta}_j - \epsilon \text{Adam}(\nabla_{\theta_j} L)$
    end for
    $X^{t+1} \leftarrow \text{Imputer}(X^t, \Omega, \hat{\Theta})$
  end for
Output: Imputations $X^{t_{\text{max}}}$, Imputer(·, ·, ·)
```

Indeed, in Algorithm 3, an imputation $\hat{X}^t, t = 0, ..., t_{\text{max}}$ is updated starting from an initial guess $X^0$. The innermost loop is dedicated to gradient-based updates of the parameter $\theta_j$. Once this inner-most loop is finished, the $j$-th variable of $\hat{X}^t$ is updated using the last update of $\theta_j$. This is then performed cyclically over all variables of $\hat{X}^t$, yielding $X^{t+1}$. In practice, several improvements on the generic Algorithms 2 and 3 can be implemented:

1. To better estimate Eq. (5), one can sample several pairs of batches (instead of a single one) and define $L$ as the average of $S_\epsilon$ divergences.

2. For Algorithm 3 in a MCAR setting, instead of sampling in each pair two batches from $X$, one of the two batches can be sampled with no missing value on the $j$-th variable, and the other with missing values on the $j$-th variable. This allows the imputations for the $j$-th variable to be fitted on actual non-missing values. This helps ensuring that the imputations for the $j$-th variable will have a marginal distribution close to that of non-missing values.

3. The order in which the variables are imputed can be adapted. A simple heuristic is to impute variables in increasing order of missing values.

4. During training, the loss can be hard to monitor due to the high variance induced by estimating Eq. (5) from a few pairs of batches. Therefore, it can be useful to define a validation set on which fictional additional missing values are sampled to monitor the training of the algorithm, according to the desired accuracy score (e.g. MAE, RMSE or $W_2$ as in Section 4).
Note that item 2 is a priori only legitimate in a MCAR setting. Indeed, under MAR or MNAR assumptions, the
distribution of non-missing data is in general not equal to
the original (unknown) distribution of missing data.\footnote{Consider as an example census data in which low/high income
people are more likely to fail to answer an income survey than
medium income people.}

4. Experimental Results

![Toy examples: 20 % missing values (MCAR) on toy datasets. Blue points have no missing values, orange points have one missing value on either coordinate. ice outputs conditional expectation imputations, which are irrelevant due to the high non-linearity of these examples. Since Algorithm 1 does not assume a parametric form for the imputations, it is able to satisfyingly impute missing values.](image)

**Baselines.** We compare our methods to three baselines:

(i) **mean** is the coordinate-wise mean imputation;

(ii) **ice** (iterative chained equations) consists in (itera-
tive) imputation using conditional expectation. Here,
we use scikit-learn’s (Pedregosa et al., 2011)
iterativeImputer method, which is based on

mice (van Buuren & Groothuis-Oudshoorn, 2011).
This is one of the most popular methods of imputation
as it provides empirically good imputations in many
scenario and requires little tuning;

(iii) **softimpute** (Hastie et al., 2015) performs missing val-
ues imputation using iterative soft-thresholded SVD’s.
This method is based on a low-rank assumption for
the data and is justified by the fact that many large ma-
trices are well approximated by a low-rank structure
(Udell & Townsend, 2019).

**New methods.** We instantiate Algorithms 1 and 3 as the
following methods:

(iv) **Sinkhorn** designates the direct non-parametric im-
putation method detailed in Algorithm 1.

For Algorithm 3, two classes of imputers are considered:

(v) **Linear RR**, i.e. in Algorithm 3, for $1 \leq j \leq d$,
Imputer($\cdot, \theta_j$) is a linear model with respect to the $d-1$
other variables with weights and biases given by $\theta_j$.
This is similar to mice or IterativeImputer,
but fitted with the OT loss eq. (5);

(vi) **MLP RR** designates Algorithm 3 coupled with shallow
Multi-Layer Perceptrons (MLP) as imputers. The fol-
lowing architecture is considered for MLP’s: (i) a first
$(d-1) \times 2(d-1)$ layer followed by a ReLU layer
then (ii) a $2(d-1) \times (d-1)$ layer followed by a
ReLU layer and finally (iii) a $(d-1) \times 1$ prediction
linear layer. All linear layers have a bias term. Each
Imputer($\cdot, \theta_j$), $1 \leq j \leq d$ is one such MLP with a
different set of weights $\theta_j$.

An additional method is presented in the appendix, which
corresponds to Algorithm 1 with a Wasserstein-Bures loss,
particular suited to elliptical distributions, which may
appear as a restrictive assumption.

**Toy experiments.** In Figure 1, we generate two-
dimensional datasets with strong structures, such as an S-
shape, half-moon(s), or concentric circles. 20% of missing
entries are introduced (void rows are discarded), and im-
putations performed using Algorithm 1 or the ice method
are compared to the ground truth dataset. While the ice method
is not able to catch the non-linear structure of the distri-
butions at all. Sinkhorn performs efficiently by imputing
faithfully to the underlying complex data structure (even
if the two half-moons and the S-shape are quite challenging).
This is remarkable, since Algorithm 1 does not rely on
any parametric assumption for the data. This underlines in
a small dimensional setting the flexibility of the proposed
method.
Figure 2: (30% MCAR) Imputation methods on 23 datasets from the UCI repository (Table 1). Sinkhorn denotes Algorithm 1 and Linear RR, MLP RR the two instances of Algorithm 3 previously described. 30% of the values are missing MCAR. All methods are evaluated on 30 random missing values draws. Error bars correspond to ± 1 std. For readability we display scaled mean $W_2$, i.e. for each dataset we renormalize the results by the maximum $W_2$. $W_2$ results for the california dataset are not displayed due to its large cardinality, which makes evaluating the unregularized $W_2$ distance difficult.

Large-scale experimental setup. We evaluate each method on 23 datasets from the UCI machine learning repository\(^3\) (see Table 1) with varying proportions of missing data and different missing data mechanisms. These datasets only contain continuous features and prior to running the experiments, the data is whitened (i.e. centered and scaled to variable-wise unit variance). For each dataset, all methods are evaluated on 30 different draws of missing values masks. For all Sinkhorn-based imputation methods, the regularization parameter $\epsilon$ is set to 5% of the median distance between initialization values with no further dataset-dependent tuning. If the dataset has more than 256 points, the batch size is fixed to 128, otherwise to $2 \lfloor \frac{n}{2} \rfloor$ where $n$ is the size of the dataset. The noise parameter $\eta$ in Algorithm 1 is fixed to 0.1. For Sinkhorn round robin models (Linear RR and MLP RR), the maximum number of cycles is 10, 10 pairs of batches are sampled per gradient update, and an $\ell^2$-weight regularization of magnitude $10^{-5}$ is applied during training. For all 3 sinkhorn-based methods, we use gradient methods with adaptive step size as per algorithms 1 and 3, with an initial step size fixed to $10^{-2}$. For Softimpute, the hyperparameter is selected at each run through cross-validation on a small grid. This CV is performed by sampling additional missing values. GPUs are used for Sinkhorn methods.\(^3\)

Metrics. Imputation methods are evaluated according to two "pointwise" metrics: mean absolute error (MAE) and root mean square error (RMSE); and one metric on distributions: the squared Wasserstein distance between empirical distributions on points with missing values. Let $X \in \mathbb{R}^{n \times d}$ be a dataset with missing values. When $(i, j)$ spots a missing entry, recall that $\hat{x}_{ij}$ denotes the corresponding imputation, and let us note $x_{ij}^\text{true}$ the ground truth. Let $m_0 \overset{\text{def}}{=} \# \{(i, j), \omega_{ij} = 0\}$ and $m_1 \overset{\text{def}}{=} \# \{ i : \exists j, \omega_{ij} = 0 \}$ respectively denote the total number of missing values and the number of data points with at least one missing value.

\(^3\)Our code is available at https://github.com/BorisMuzellec/MissingDataOT
Figure 3: (30% MNAR) Imputation methods on 23 datasets from the UCI repository (Table 1). Values are missing MNAR according to the logistic mechanism described in Section 4, with 30% variables used as inputs of a logistic masking model for the remaining 70% remaining variables. Those input variables are then masked at 30% at random. Hence, all variables have 30% missing values. All methods are evaluated on 30 random missing values draws. Error bars correspond to ±1 std. For readability we display scaled mean $W^2$, i.e. for each dataset we renormalize the results by the maximum $W^2$. Results for the california dataset are not displayed due to its large cardinality, which makes evaluating the unregularized $W^2$ distance difficult.

Set $M_1 \eqdef \{i : \exists j, \omega_{ij} = 0\}$. We define MAE, RMSE and $W^2$ imputation metrics as

\[
\frac{1}{m_0} \sum_{(i,j) : \omega_{ij} = 0} |x_{ij}^{true} - \hat{x}_{ij}|, \quad \text{(MAE)}
\]

\[
\sqrt{\frac{1}{m_0} \sum_{(i,j) : \omega_{ij} = 0} (x_{ij}^{true} - \hat{x}_{ij})^2}, \quad \text{(RMSE)}
\]

\[
W^2 \left( \mu_{m_1} \left( \mathbf{X}_{M_1} \right), \mu_{m_1} \left( \mathbf{X}_{M_1}^{(true)} \right) \right). \quad \text{(W2)}
\]

**Missing value generation mechanisms.** The implementation of a MCAR mechanism is straightforward. On the contrary, many different mechanisms can lead to a MAR or MNAR setting. We here describe those used in our experiments. In the MCAR setting, each value is masked according to the realization of a Bernoulli random variable with a fixed parameter. In the MAR setting, for each experiment, a fixed subset of variables that cannot have missing values is sampled. Then, the remaining variables have missing values according to a logistic model with random weights, which takes the non-missing variables as inputs. The outcome of this logistic model is re-scaled to attain the desired proportion of missing entries. Finally, two different mechanisms are implemented in the MNAR setting. The first is identical to the previously described MAR mechanism, but the inputs of the logistic model are then masked by a MCAR mechanism. Hence, the logistic model’s outcome now depends on potentially missing values. The second mechanism samples a subset of variables whose values in the lower and upper $p$-th percentiles are masked according to a Bernoulli random variable, and the values in-between are left not missing.

**Results.** Results are reported in Figure 2 and Figure 3. For the direct imputation method Algorithm 1, results with 10% and 50% missing values and under the MAR and MNAR mechanisms described above are presented in the Appendix. As can be seen from Figure 2, the linear round-robin model
matches or out-performs scikit’s iterative imputer (ice) on MAE and RMSE scores for most datasets. Since both methods are based on the same cyclical linear imputation model but with different loss functions, this shows that the batched Sinkhorn loss in Eq. (5) is well-adapted to imputation with parametric models. Interestingly, while the MAE and RMSE scores of the round robin MLP model are comparable to that of the linear RR, its $W^2$ scores are generally quite better. This suggests that more powerful base imputer models lead to better $W^2$ scores, from which one can conclude that Eq. (5) is a good proxy for optimizing the unavailable Eq. (1) score, and that Algorithm 3 is efficient at doing so. Furthermore, one can observe that the direct imputation method is very competitive over all data and metrics and is in general the best performing OT-based method, as could be expected from the fact that its imputation model is not restricted by a parametric assumption. This favorable behaviour tends to be exacerbated with a growing proportion of missing data, see Figure 6 in the appendix.

**Out-of-sample imputation.** As mentioned in Section 3, a key benefit of fitting a parametric imputing model with algorithms 2 and 3 is that the resulting model can then be used to impute missing values in out-of-sample (OOS) data. In Figure 4, we evaluate the Linear RR and MLP RR models in an OOS imputation experiment. We compare the training and OOS MAE, RMSE and OT scores on a collection of datasets selected to have a sufficient number of points. At each run, we randomly sample 70% of the data to be used for training, and the remaining 30% to evaluate OOS imputation. 30% of the values are missing MCAR accross both training and testing sets.

**MAR and MNAR.** Figure 3 displays the results of our experiments in a MNAR setting, and shows that the proposed methods are robust to difficult missing mechanisms. Additional experiments with MAR and different MNAR mechanisms are deferred to the Appendix.

**Conclusion.** We have shown in this paper how OT metrics could be used to define a relevant loss for missing data imputation. This loss corresponds to the expectation of Sinkhorn divergences between randomly sampled batches. To minimize it, two classes of algorithms were proposed: one that freely estimates one parameter per imputed value, and one that fits a parametric model. After training, this latter class allows out-of-sample imputation. To make parametric models trainable, the classical round robin mechanism was used. Experiments on a variety of datasets, and for numerous missing value settings (MCAR, MAR and MNAR with varying missing values proportions) showed that the proposed models are very competitive, and confirmed that our loss is a good optimizable proxy for imputation metrics. Future work includes further theoretical study of our loss function Eq. (5) within the OT framework, and exploiting the flexibility of algorithms 2 and 3 to design new imputers.
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A. Appendix

In this appendix, additional experimental results are presented. These results correspond to the missing value mechanisms described in Section 4:

1. 10% MCAR (Figure 5) and 50% MCAR (Figure 6);
2. 30% MAR on 70% of the variables with a logistic masking model (Figure 7);
3. 30% MNAR generated with a logistic masking model, whose inputs are then themselves masked (Figure 8);
4. 30% MNAR on 30% of the variables, generated by censoring upper and lower quartiles (Figure 9).

These experiments show that the proposed methods are robust to different levels of noise, as well as to MAR and MNAR mechanisms.

Code. Our code is available in the following anonymized repository: https://github.com/BorisMuzellec/MissingDataOT.
Figure 5: (10\% \textbf{MCAR}) Imputation methods on 23 datasets from the UCI repository (Table 1). 10\% of the values are missing MCAR. All methods are evaluated on 30 random missing values draws. Error bars correspond to $\pm$ 1 std. For better readability we display scaled mean $W_2$, i.e. for each dataset we renormalize the results by the maximum mean $W_2$. Results for the \texttt{california} dataset are not displayed due to its large cardinality, which makes evaluating the $W_2$ distance difficult (but not training with $S_\epsilon$).
Figure 6: (50 % MCAR) Imputation methods on 23 datasets from the UCI repository (Table 1). 50% of the values are missing MCAR. All methods are evaluated on 30 random missing values draws. Error bars correspond to $\pm 1$ std. For better readability we display scaled mean $W_2^2$, i.e. for each dataset we renormalize the results by the maximum mean $W_2^2$. $W_2$ results for the **california** dataset are not displayed due to its large cardinality, which makes evaluating the $W_2$ distance difficult (but not training with $S_\varepsilon$).
Figure 7: (30% MAR: log) Imputation methods on 23 datasets from the UCI repository (Table 1). Values are missing MNAR according to the logistic mechanism described in Section 4, with 30% variables used as inputs of a logistic masking model for the remaining 70% remaining variables. Those input variables are then masked at 30% at random. Hence, all variables have 30% missing values. All methods are evaluated on 30 random missing values draws. Error bars correspond to ±1 std. For readability we display scaled mean $W_2^2$, i.e. for each dataset we renormalize the results by the maximum $W_2^2$. $W_2$ results for the california dataset are not displayed due to its large cardinality, which makes evaluating the unregularized $W_2$ distance difficult.)
**Figure 8:** (30% MNAR: log) Imputation methods on 23 datasets from the UCI repository (Table 1). Values are missing MNAR according to the logistic mechanism described in Section 4, with 30% variables used as inputs of a logistic masking model for the remaining 70% remaining variables. All variables have 30% missing values (MNAR or MCAR for the input variables). All methods are evaluated on 30 random missing values draws. Error bars correspond to ± 1 std. For better readability we display scaled mean $W^2$, i.e. for each dataset we renormalize the results by the maximum mean $W^2$. $W^2$ results for the california dataset are not displayed due to its large cardinality, which makes evaluating the $W^2$ distance difficult (but not training with $S_e$).
Figure 9: (MNAR; quantile) Imputation methods on 23 datasets from the UCI repository (Table 1). Values are missing MNAR according the quantile censoring mechanism described in Section 4, with 30% of the variables having 30% missing values in their first and last quartiles. All methods are evaluated on 30 random missing values draws. Error bars correspond to ± 1 std. For better readability we display scaled mean $W_2$, i.e. for each dataset we renormalize the results by the maximum mean $W_2$. $W_2$ results for the california dataset are not displayed due to its large cardinality, which makes evaluating the $W_2$ distance difficult (but not training with $S_0$).