

Rethinking the Diffusion Models for Missing Data Imputation: A Gradient Flow Perspective

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Background Introduction

- 1.1 Missing Data Imputation (MDI) Task
- (1) Suppose we have an **ideal tabular data**: $X^{(ideal)} \in \mathbb{R}^{N \times D}$.
- \hat{Q} However, at hand, we have an **observational data** : $X^{(obs)} =$ $X^{(ideal)} \bigodot M + \text{NaN} \bigodot (\mathbf{1}_{N \times D} - M).$
- **③** Where NaN is the abbreviation of **not a number**, $M \in \{0,1\}^{N \times D}$ is **mask matrix**, and $\mathbf{1}_{N\times D}$ is the **matrix of ones**.
- $\textcircled{4}$ We should **recover** $X^{\text{(ideal)}}$ by imputation matrix $X^{\text{(imp)}}$ as follows: $\widehat{X} = X^{(\text{ideal})} \odot M + X^{(\text{imp})} \odot (1_{N \times D} - M).$

Background Introduction

- 1.2 Diffusion Model for Missing Data Imputation ① Suppose we have a **score function**: $\overline{V}_X \log p(X)$
- (2) Diffusion models generate samples by simulating the SDE: $dX_{\tau} =$ $f(X_\tau) d\tau + g_\tau dW_\tau$
- $\textcircled{3}$ Where τ is the time, $f(X_{\tau})$ is **drift term,** which is **concerned with score function,** g_{τ} is the **volatility term**. The **density** $r(X_{\tau})$ is **governed by:** $\frac{\partial r(X_{\tau})}{\partial \tau}$ $\frac{d\Gamma(X_{\tau})}{d\tau} = -\nabla \cdot \left(r(X_{\tau})f(X_{\tau})\right) + \frac{1}{2}g_{\tau}^2 \nabla \cdot \nabla r(X_{\tau})$
- ④ Diffusion-Model-based MDI treats the MDI problem as a conditional generative problem, which aims to generate samples from **conditional score function**: $\nabla_{\mathbf{x}(\text{miss})} \log p(\mathbf{X}^{(\text{miss})} | \mathbf{X}^{(\text{obs})})$
- ⑤ In practice, ground-truth missing values are unavailable, thus, we should **mask part of data** to construct the score function: $\nabla_{\mathbf{x}(\text{miss})} \log p(\mathbf{X}^{(\text{miss})} | \mathbf{X}^{(\text{obs})}).$

Background Introduction

1.3 Wasserstein Gradient Flow

- Suppose we want to optimize a **cost functional**: \mathcal{F}_{cost} : $\mathcal{P}_2(\mathbb{R}^D) \to \mathbb{R}$
- Wasserstein Gradient Flow is an absolute continuous trajectory $(q_{\tau})_{\tau \geq 0}$, that descend $\mathcal{F}_{\text{cost}}$ as effective as possible.
- ③ The trajectory in Wasserstein Gradient Flow is governed by the **continuity equation**: $\frac{\partial u}{\partial \tau} = -V \cdot (u_\tau q_\tau)$
- **4 Velocity field** u_{τ} is given by $u_{\tau} = -\nabla_X \frac{\delta \mathcal{F}_{cost}}{\delta q_{\tau}}$ δq_{τ} .
- ⑤ Based on this, the evolution of ∈ ℝDcan be **delineated by the ODE** $\frac{dX_{\tau}}{d\tau}$ $\frac{c}{d\tau} = u_{\tau}$

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Motivation

2.1 The Task for MDI: An Optimization Perspective

Based on the **Maximum Likelihood Estimation principle**, we can obtain the following optimization problem:

 $X^{(\text{imp})} = \text{argmax}_{X^{(\text{miss})}} \log \hat{p}(X^{(\text{miss})}|X^{(\text{obs})}).$

From the perspective of **probabilistic machine learning**, we can reframe the following cost functional:

 $\argmax_{r(X^{(\text{miss})})} \mathbb{E}_{r(X^{(\text{miss})})} \big[\log \hat{p}(X^{(\text{miss})} | X^{(\text{obs})}) \big],$

where we assume that $X^{(miss)}$ comes from a proposal distribution $r(X^{(miss)})$, optimizing the sample $X^{(miss)}$ is optimizing the distribution.

Motivation

2.2 A Toy Case for DM-based Optimization

Suppose we have a Dirichlet distribution supports on Δ^2 , and we want to optimize the functional defined as follows:

$$
\text{argmax}_{\mathbf{a}_h \in \Delta^2} \sum_{h=1}^H \{ \log \left(\frac{\Gamma(\sum_{k=1}^3 \rho_k)}{\prod_{k=1}^3 \Gamma(\rho_k)} \right) + \sum_{k=1}^3 (\rho_k - 1) \log \mathbf{a}_{k,h} \},
$$

where a_h is the variable, $\rho_k|_{k=1}^3 = [2.5,2.5,5.0]$ is concentration parameter, and H is the sample number.

Motivation

2.2 A Toy Case for DM-based Optimization

Expected Optimal Results Results by Diffusion Models

The results tend to **cluster around** the expected optimal results

- There might be something **implicitly optimized** during DMs
- And this **implicitly optimized** term may result in **diversity**

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- 3.1 What makes a diversified imputation result?
- ① d $X_{\tau} = f(X_{\tau})d\tau + g_{\tau}dW_{\tau}$ is governed by $\frac{dr(X_{\tau})}{\partial \tau}$ $= -V$ $r(X_{\tau})f(X_{\tau}) + \frac{1}{2}g_{\tau}^2 \nabla \cdot \nabla r(X_{\tau}).$
- ② The trajectory in Wasserstein Gradient Flow is governed by the **continuity equation**: $\frac{\partial}{\partial \tau} = -V \cdot (u_\tau q_\tau)$

Let us **analyze and improve** the diffusion model-based MDI within the Wassersetin gradient flow framework!

3.1 What makes a diversified imputation result?

- For diffusion model-based MDI, we can find that they are optimizing the following cost functional: $argmax_{r(X^{(miss)})} \mathbb{E}_{r(X^{(miss)})} [log \hat{p}(X^{(miss)}|X^{(obs)})] + \psi(X^{(miss)}) + const$
- **• VP-SDE:** $\psi(X^{(\text{miss})}) = \frac{1}{2}$ $\frac{1}{2} \mathbb{H} \left[r \left(\boldsymbol{X}^{(\text{miss})} \right) \right] + \frac{1}{4} \mathbb{E}_{r \left(\boldsymbol{X}^{(\text{miss})} \right)} \left\{ \left[\boldsymbol{X}^{(\text{miss})} \right]^\mathsf{T} \left[\boldsymbol{X}^{(\text{miss})} \right] \right\} \geq 0$
- **• VE-SDE:** $\psi(X^{(\text{miss})}) = \frac{1}{2}$ $\frac{1}{2}$ $\mathbb{H}\left[r(X^{(\text{miss})})\right] \geq 0$
- **sub-VP-SDE:** $\psi(X^{(\text{miss})}) = \frac{1}{2} \mathbb{H} \left[r(X^{(\text{miss})}) \right] + \frac{1}{4\gamma_{\tau}} \mathbb{E}_{r(X^{(\text{miss})})} \left\{ \left[X^{(\text{miss})} \right]^{\top} \left[X^{(\text{miss})} \right] \right\} \geq 0$
- $w(X^{(\text{miss})})$ consistently **greater than 0**.
- **Entropy** term $\frac{1}{2}$ 2 $\mathbb{H}\left[r(X^{(miss)})\right]$ results in **diversity**.

3.2 How to eliminate the diversity?

- $\triangleright \psi(X^{(\text{miss})})$ should be **smaller than 0**.
- The design regularized term should **eliminate diversity**.
- The **negative entropy** is a suitable choice:

$$
\psi\big(X^{(\text{miss})}\big) = -\lambda \mathbb{H}\big[r\big(X^{(\text{miss})}\big)\big], \lambda \geq 0
$$

 \triangleright We can define a novel cost functional as follows:

$$
\mathcal{F}_{\text{NER}} = \mathbb{E}_{r(X^{(\text{miss})})} \left[\log \hat{p}(X^{(\text{miss})} | X^{(\text{obs})}) \right] - \lambda \mathbb{H} \left[r(X^{(\text{miss})}) \right]
$$

 We call our approach termed '**N**egative **E**ntropy-regularized **W**asserstein Gradient Flow-based **Imp**utation', aka, **NewImp**.

3.3 How to optimize this functional?

 \triangleright Within WGF framework, we can optimize the \mathcal{F}_{NFR} with the help of the following velocity field:

$$
u(X^{(\text{miss})}) = -\nabla_{X^{(\text{miss})}} \frac{\delta \mathcal{F}_{\text{NER}}}{\delta r(X^{(\text{miss})})}
$$

$$
= \nabla_{X^{(\text{miss})}} \log \hat{p}(X^{(\text{miss})} | X^{(\text{obs})}) + \lambda \nabla_{X^{(\text{miss})}} \log r(X^{(\text{miss})})
$$

However, implementing this velocity filed to obtain imputed value by $\frac{dX^{(miss)}}{dx}$ $d\tau$ $= u(X^{(miss)})$ requires explicitly estimating intractable density function $r(X^{(miss)})$:

- \triangleright Directly estimating $r(X^{(miss)})$ is intractable.
- Analytically solving the continuity equation $\frac{\partial r(X^{(miss)})}{\partial \tau}$ $\boldsymbol{\theta}$ $=-V$ \cdot $\lceil u(X^{(\text{miss})})r(X^{(\text{miss})}) \rceil$ is **difficult**.

3.3 How to optimize this functional?

Fortunately, with the help of the following two conditions, we can realize the velocity filed in computer language:

- ① Velocity filed is restricted within the RKHS satisfies the boundary condition: $u(X^{(miss)}) \in K(X^{(miss)}, X^{(miss)})$, and the kernel function satisfies: $\lim_{n \tilde{\mathbf{v}}(\text{miss})}$ $\|\tilde{X}^{(\text{miss})}\| \to \infty$ $K(X^{(\text{miss})}, \bar{X}^{(\text{miss})}) = 0.$
- 2 Density function $r(X^{(miss)})$ is bounded.

We can get:

$$
u(X^{(\text{miss})})\n= \mathbb{E}_{r(\widetilde{X}^{(\text{miss})})}\n\left\{\n\begin{array}{c}\n-\lambda \nabla_{\widetilde{X}^{(\text{miss})}} K(X^{(\text{miss})}, \widetilde{X}^{(\text{miss})}) \\
+\left[\nabla_{\widetilde{X}^{(\text{miss})}} \log \hat{p}(\widetilde{X}^{(\text{miss})} | X^{(\text{obs})})\right]^{\top} K(X^{(\text{miss})}, \widetilde{X}^{(\text{miss})})\n\end{array}\n\right\}
$$

3.4 Can we sidestep the mask modeling?

Interestingly, we can find another joint distribution related costfunctional:

$$
\mathcal{F}_{joint-NER} = \mathbb{E}_{r(X^{(joint)})} [\log \hat{p}(X^{(joint)})] - \lambda \mathbb{H}[r(X^{(joint)})]
$$

We can prove that:

$$
\triangleright \quad \mathcal{F}_{joint-NER} = \mathcal{F}_{NER} - const
$$

 Within Wasserstein gradient flow framework, the **velocity filed induced by** $\mathcal{F}_{joint-NER}$ is **identity to** the velocity filed induced by $\mathcal{F}_{\text{NER}}, u(X^{(\text{joint})})$ satisfies: $u(X^{(\text{joint})}) = u(X^{(\text{miss})}).$

- 3.4 Can we sidestep the mask modeling? By far, we merely need to simulate the velocity field: $u(X^{(joint)})$ $=\mathbb{E}_{r(\widetilde{X}^{(\text{joint})})}$ $-\lambda \nabla_{\widetilde{\boldsymbol{X}}^{(\text{miss})}} K\big(\boldsymbol{X}^{(\text{joint})},\widetilde{\boldsymbol{X}}^{(\text{joint})}\big)$ $+ \big[\nabla_{\widetilde{\boldsymbol{X}}^{(\text{miss})}} \log \hat{p}(\widetilde{\boldsymbol{X}}^{(\text{joint})}) \big]^\top K\big(\boldsymbol{X}^{(\text{joint})}, \widetilde{\boldsymbol{X}}^{(\text{joint})} \big)$ We concerning terms can be realized by:
	- \triangleright $K(X^{(joint)}, \widetilde{X}^{(joint)}) = \exp(-\frac{\|X^{(joint)} \widetilde{X}^{(joint)}\|_2^2}{2h^2})$ $\frac{1}{2h^2}$
- $\triangledown_{\widetilde{X}^{(\text{miss})}} K(X^{(\text{joint})}, \widetilde{X}^{(\text{joint})}) = \nabla_{\widetilde{X}^{(\text{joint})}} K(X^{(\text{joint})}, \widetilde{X}^{(\text{joint})}) \bigodot (\mathbf{1}_{N \times D} \mathbf{1}_{N \times D})$ $(M) + 0 \times M$
- $\triangleright \quad \nabla_{\widetilde{X}^{(\text{miss})}} \log \hat{p}(\widetilde{X}^{(\text{joint})}) = \nabla_{\widetilde{X}^{(\text{joint})}} \log \hat{p}(\widetilde{X}^{(\text{joint})}) \bigcirc (\mathbf{1}_{N \times D} M) + 0 \times M$
- \triangleright $\mathbb{E}_{r(\tilde{X}^{(joint)})}$ realized by Monte Carlo approximation
- Now we **merely remain the implementation** of $\nabla_{\widetilde{\mathbf{x}}^{(joint)}} \log \hat{p}(\widetilde{\mathbf{X}}^{(joint)})$.

3.4 Estimation of Joint Distribution

Up to now, our primary task is to estimate the joint distribution $\nabla_{\boldsymbol{\mathit{X}}}$ (joint) $\log \hat{p}(\boldsymbol{\mathit{X}}^{(\text{joint})}).$

- We parameterize the score function $\nabla_{\mathbf{x}^{(joint)}} \log \hat{p}(\mathbf{x}^{(joint)})$ by a neural network.
- \triangleright The neural network is trained by denoise score matching (DSM) by the following loss function:

$$
\mathcal{L}_{DSM} = \frac{1}{2} \mathbb{E}_{q_{\sigma}(\hat{X}^{(joint)}|X^{(joint)})} [\|\nabla_{\hat{X}^{(joint)}} \log \hat{p}(\hat{X}^{(joint)}) - \nabla_{\hat{X}^{(joint)}} \log q_{\sigma}(\hat{X}^{(joint)}|X^{(joint)})\|^{2}]
$$

\n
$$
\triangleright \text{ where } \hat{X}^{(joint)} = X^{(joint)} + \epsilon, \epsilon \sim \mathcal{N}(0, \sigma^{2} I)
$$

3.5 Overall Framework

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Experimental Results

(b) Student's- t

4.1 Toy Case Study Results

(a) Standard Gaussian

- \triangleright NewImp approach outperforms on different types of data.
- \triangleright This phenomenon reflects that the NewImp approach is robust to data type like heavy-tailed, skewed, and multi-modal.

Experimental Results

4.2 Baseline Comparison

Kindly Note: The best results are **bolded** and the second best results are underliend. "*" marks the results that NewImp significantly outperform with p -value < 0.05 over paired samples t-test.

NewImp approach outperforms most of prevalent models.

Experimental Results

4.3 Ablation Study

Kindly Note: The best results are **bolded** and the second best results are *underliend*. "*" marks the results that NewImp significantly outperform with p -value < 0.05 over paired samples t-test.

 Both of the negative regularization term and joint modeling strategy are effective for model performance improvement.

Thank you for listening! All suggestions are welcomed. !