Meta-learning Implicit Neural Representation for Sparse Time Series Functional Data Analysis

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Abstract

Sparse time series data is everywhere in our daily life. However it is hard to analyze them by traditional statistical methods. Here, we propose MetaINR, a method to learning the implicit neural representation (INR) of time series given sparse and irregular obsevations. Based on MetaINR, estimations of mean function, covariance operator, and principal components can be implemented easily. The method introduce the meta-learning to the functional data analysis (FDA) framework, which greatly outperforms the traditional baseline.

1 Introduction

Sparse time series data is common in daily life, such as medical data measured at different times for patients or height data collected at various stages of adolescence. However, the sparsity and irregularity of such data make traditional statistical methods hard to apply directly. Additionally, the consideration of continuity and differentiability properties in most time series data pose challenges for multivariable statistical analysis.

Recent research suggests that meta-learning exhibits great advantages in handling sparse data. It can learn commonalities among similar tasks, enabling few-shot learning or even one-shot learning on extremely sparse training sets. Besides, statistical analysis based on dense functional data has been hugely developed for dealing with continuous time series problems.

In this paper, we introduce a novel approach, MetaINR, which combines meta-learning and functional data analysis to address the estimation challenges posed by sparse time series data. Through this method, we use meta-learning to realize the implicit neural representation (INR) to reconstruct the time series function for each sample based on sparse time series observations. Furthermore, we can estimate the mean, covariance, and principal components of the distribution behind these samples. The advantange of MetaINR can be summarized as follows:

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Therefore, MetaINR method presents a new solution for addressing issues related to sparse time series data.

2 Related works

2.1 Functional Data

[TODO: add references]

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Multivariate data versus functional data Traditional multivariate statistics take finite-dimensional vectors as the objects of study to analyze their statistical properties, such as mean vectors and covariance matrices. This approach is appropriate and is easy to compute when the dimension of the statistical objects is relatively small. However, if the dimension of the space is increased to infinite, for example, in L^2 space, traditional methods face certain challenges. Besides the expensive computational cost, in such functional spaces, people's focus is not only on the values of vectors in a particular dimension but also on properties such as continuity, smoothness and derivatives. Additionally, as the space grows to infinite dimensions, many useful tools in multivariate statistics, such as probability density functions, will lose their meaning. It is the differences in statistical properties and people's focus between infinite-dimensional and finite-dimensional spaces, that have led to widespread attention to functional data analysis (FDA) among researchers. In FDA, scientists treat functions as basic elements for analysis and have developed various methods to estimate the statistical properties for a functional distribution, such as mean function, covariance operator and functional principal components.

Time series as a representative example of functional data Time series is a typical object that needs to be addressed in an infinite-dimensional function space. This is because time series data collected in reality often exhibit continuity, and, in certain situations, people may focus on topics such as derivatives and time alignment (registration). Many previous studies have relied on multivariate statistics in the analysis of time series, such as [mention some specific examples]... From the perspective of function approximation, these multivariate-statistics-based studies can indeed reflect certain properties of time series. However, in many cases, this approach is challenging to generalize, as is the case with sparse time series data studied in this paper.

Sparse times series data analysis When the observation frequency of time series is low and irregular, sparse time series data is formed. We can represent the sparse dataset of n samples as

$$D = \{(t_{ij}, y_{ij})_{j=1}^{J}\}_{i=1}^{n}$$

where $y_{ij} = x_i(t_{ij}), i = 1, \cdots, n, j = 1, \cdots, J_i$ and J_i is the total observations of the i-th sample. This type of data is particularly common in the medical field, as the frequency of medical visits varies from person to person, with irregular patterns. When it comes to analyzing such "messy" data using multivariate statistics, people often find themselves at a loss. However, in functional data analysis, one can employ the method of local polynomial regression to estimate the mean function and covariance operator of functional data. Specifically, given our sparse observations of dataset D, we can define the loss function to estimate mean function $\mu(t)$

$$L_t^{\mu}(\beta) = \sum_{i=1}^{n} \sum_{j=1}^{J_i} \left[y_{ij} - \sum_{r=0}^{R} \beta_r \left(t - t_{ij}\right)^r \right]^2 K\left(\frac{t - t_{ij}}{h}\right),$$

where $K(\cdot)$ is the kernel function and h is the bandwidth which shoud be carefully chosen based on data. By minimizing this function, we can get $\beta_t = (\beta_0(t), \cdots, \beta_R(t)) = arg\,min L_t^{\mu}(\beta)$. The estimator of mean function cam be defined as $\hat{\mu}(t) = \beta_0(t)$. Similarly, to estimate the covariance kernel $c(t, s)$, we define the loss function

$$L_{t,s}^{c}(\beta) = \sum_{i=1}^{n} \sum_{1 \le j,l, \le J_i} K_{t,s}(\frac{t - t_{ij}}{h}, \frac{s - t_{il}}{h}) \left[g(t_{ij}, t_{il}) - f\left(\beta, (t, s), (t_{ij}, t_{il})\right)\right]^2$$

where

$$g(t_{ij}, t_{il}) = (y_{ij} - \hat{\mu}(t_{ij}))(y_{il} - \hat{\mu}(t_{il}))$$
$$f\left(\beta, (t, s), (t_{ij}, t_{il})\right) = \beta_0 + \beta_{11}(t - t_{ij}) + \beta_{12}(s - t_{il})$$

By minimization of $L_{t,s}^{c}(\beta)$, we obtain $(\beta_0(t), \beta_{11}(t), \beta_{12}(t)) = arg\,min L_{t,s}^{c}(\beta)$. Then the estimator of the covariance kernel is defined as $\hat{c}(t, s) = \beta_0(t, s)$. Based on the estimation of mean and covariance, we can use the method of Principal Analysis by Conditional Expectation (PACE) to reconstruct each sample and compute their scores (see details in the appendix)[TODO].

The drawbacks of traditional FDA method for sparse data Comparing to using local polynomial regression directly to reconstruct samples, It is noticeable that the reconstruction of the sample in this method makes use of the total of information of all observations, but it hugely relies on the assumption that scores are normally distributed. In the following text, I will compare the estimates obtained based on this method as the baseline with the meta-learning-based approach proposed in this paper.[TODO PACE baseline coding]

2.2 Implicit Neural Representation

Traditional grid-based representation versus implicit neural representation Traditionally, the representation of functional data $y(t)$ involves using a standard grid-based method, wherein a finite set of coordinates and corresponding function values are given as pairs (t_i, y_i). However, this approach has certain drawbacks: the original functional data in an infinite-dimensional space is discretized into a finite-dimensional space. This not only hampers operations like differentiation but also significantly impacts the resolution of the function within a smaller time interval. With the emergence of deep learning, it has been discovered that utilizing deep neural networks can be an effective way to represent functions implicitly. Implicit neural representation (INR) parameterize the functional data by deep neural networks:

$$y(t) = F_\phi(t),$$

where $F_\phi(\cdot)$ is a deep neural network parameterized by ϕ. This type of continuous representation not only proves to be more memory-efficient but also enables higher resolution and the handling of more complex operations on functional data.

SIREN architecture for time series Many prior works have utilized ReLU-based multilayer perceptrons (MLP) as the neural network architecture for Implicit Neural Representations (INR). However, ReLU-based INR often lack the ability to capture fine details in signal and struggle to effectively express higher-order derivatives. In addressing this limitation, [1] introduced the SIREN architecture as an alternative to traditional ReLU-MLPs:

$$\Phi(\mathbf{x}) = \mathbf{W}_n \left(\phi_{n-1} \circ \phi_{n-2} \circ \ldots \circ \phi_0\right)(\mathbf{x}) + \mathbf{b}_n, \quad \mathbf{x}_i \mapsto \phi_i\left(\mathbf{x}_i\right) = \sin\left(\mathbf{W}_i \mathbf{x}_i + \mathbf{b}_i\right)$$

SIREN employs the sine function as the activation function, effectively capturing intricate details in functions. A remarkable observation is that even after taking derivatives of a function represented using SIREN, it can still be expressed using the SIREN architecture. While previous research predominantly applied SIREN to represent images and videos, its application in time series representation has been limited.

The advantages of SIREN-based INR for further functional analysis This paper explores the utilization of SIREN in the analysis of time series and demonstates its superiority in time series INR.

2.3 Meta-learning

Meta-learning framework Meta-learning was initially introduced to enhance the efficiency of machine learning, often referred to as "learning to learn". By employing the deep learning model $F_\phi(\cdot)$ to address similar tasks, the "shared characteristics" among these tasks can be leveraged to expedite the machine learning process. To fomulate, given the observation dataset D^* of the target task and the observation dataset $D = \bigcup_{i=1}^n D_i$ of n similar tasks, we need to find a meta-function to effectively learn the parameters of the given task, namely $\phi^* = f_\theta(D, D^*)$, where θ is the meta-parameter of the meta-function $f_\theta(\cdot)$. Accordingly, the original target task can be solved as $F_{\phi^*}(\cdot)$. In fact, the representation of meta-function $f_\theta(\cdot)$ can be diverse. There are two main classes of methods: Parameterized Policy Gradient Methods (PPG) and Black Box Methods.

Parameterized Policy Gradient Methods and MAML The PPG method use an iterative algorithm to represent f_θ, which has an innerloop of the form:

$$\phi^*_{j+1} = \phi^*_j - \alpha_\theta \nabla_{\phi^*_j} \hat{L}_\theta \left(D^*, F_{\phi^*_j}\right),$$

with the initial value $\phi^*_0 = \phi^*_0(\theta)$. This is very intuitive because it is similar to the traditional gradient decent method to optimize. The only difference is that θ should be carefully determined by the observations of other tasks D in this scenario. One important example of PPG method is MAML, where $\phi^*_0(\theta) = \theta$ and $\hat{L}_\theta$ can be any loss function independent of θ. MAML can be regarded as learning an initial value for a task distribution, which retains the gradient decent framework of traditional optimization algorithms.

Black box methods Since we only care about the target function $F_\phi(\cdot)$ rather than the value of parameters ϕ, an alternative way to treat $f_\theta(\cdot)$ is to see it as a black box. Based on this idea, we can rewrite the target function:

$$F_\phi(t) = F_{f_\theta(D, D^*)}(t) = g_\theta(t, D, D^*)$$

Here we do not need to explicitly specify the value of ϕ, and treat the meta-learning task as another "big" task, which adds all the training materials into input.

PPG versus black box methods For black box methods, because of the sequential properties of the datasets, sequential model architectures such as RNN are used in g_θ, which unavoidably change the initial architecture F_ϕ. In contrast, PPG methods use the meta-parameters θ to find the task parameters ϕ explicitly, which maintain the initial network architecture. Therefore, black box methods have inductive bias from data while PPG methods have inductive bias in network structure. In the context of time series Implicit Neural Representation (INR), selecting an appropriate network structure is crucial, as it directly influences properties such as continuity and differentiability. Hence, in this paper, we opt for MAML as our meta-learning method for the INR task.

2.4 Other learning method for sparse data INR

3 Method

[picture, illustration]

Overview of MetaINR Given sparse observations of n similar time series, the goal of MetaINR is to reconstruct each sample as accurately as possible and identify the principal components (PC) of the distribution behind these time series. Here, we choose an alternative way by using the method of meta-learning, which involves three main steps:

- Learning the meta-model: use SIREN architecture and MAML algorithm to learn the meta-model for the INR of given time series.
- Recovery of samples: calculate the SIREN-based INR efficiently for each time series sample based on the mata-model.
- Functional data estimation: use MetaINR of each sample to estimate the mean function, covariance kernel and principal components.

We now discuss each step.

Learning the meta-model The tasks here are realizing the implicit neural representation of samples by the SIREN architecture $F_\phi(t)$. Given the sparse observations of n similiar time series $D = \{(t_{ij}, y_{ij})_{j=1}^{J_i}\}_{i=1}^n$, we use MAML algorithm 1 to learning the meta-model of these tasks, whose initial value of parameters are denoted by ϕ_0. The MAML optimization process to find ϕ_0 can be expressed as follows:

Recovery of samples Based on this meta-model, we can use gradient decent algorithm2 to calculate the optimal parameters ϕ_i^* for the sample i and hence obtain the INR $F_{\phi_i^*}(t)$.

Functional data estimation Based on the estimated INR $\hat{y}_i(t) = F_{\phi_i^*}(t)$, we subsequently estimate the mean function $\hat{\mu}(t)$ and covariance kernel $\hat{c}(t,s)$ as follows:

$$\hat{\mu}(t) = \frac{1}{n}\sum_{i=1}^{n}\hat{y}_i(t)$$

$$\hat{c}(t,s) = \frac{1}{n}\sum_{i=1}^{n}[\hat{y}_i(t)) - \hat{\mu}(t)][\hat{y}_i(s) - \hat{\mu}(s)]$$

According to the covariance operator, we can further estimate its principal components $\hat{\phi}_k$ by calculate the eigenfunctions of $\hat{c}(t,s)$.

Discussion (motivation, advantage) As discussed in the previous section, in traditional approaches, we first use local polynomial regression to estimate the mean and covariance of these time series. Under the assumption that scores follow a normal distribution, the PACE method can then be employed to estimate each principal component and reconstruct each sample. While this two-step estimation method is indeed superior to directly reconstructing samples using local polynomials as it leverages information from all samples, it still has the notable drawback that the assumption of normal-distributed scores is too restrictive.

Algorithm 1 Model-Agnostic Meta-Learning for Time Series Implicit Neural Representation

Input: $D = \{(t_{ij}, y_{ij})_{j=1}^{J_i}\}_{i=1}^{n}$: the sparse observations for tasks
Input: α, β : step size hyperparameters
  randomly initialize θ
  while not done **do**
    for all i **do**
      $\theta^0 \leftarrow \theta$
      for $q = 0$ to $Q - 1$ **do**
        Evaluate $\nabla_{\theta^q} \mathcal{L}_i \left(F_{\theta^q}\right)$ using support set $D_i^{\text{support}} = (t_{ij}, y_{ij})_{j=1}^{\lfloor 0.5 * J_i \rfloor}$
        Compute adapted parameters with gradient descent: $\theta_i^{q+1} = \theta_i^q - \alpha \nabla_{\theta_i^q} \mathcal{L}_i \left(F_{\theta_i^q}\right)$
      end for
      Compute the loss $\mathcal{L}_i \left(F_{\theta_i^Q}\right)$ in sample i using query set $D_i^{\text{query}} = (t_{ij}, y_{ij})_{j=\lfloor 0.5 * J_i \rfloor}^{J_i}$
    end for
    Compute the total loss $\mathcal{L} = \sum_{i=1}^{n} \mathcal{L}_i \left(F_{\theta_i^Q}\right)$
    Update meta-parameters $\theta \leftarrow \theta - \beta \nabla_\theta \mathcal{L}$
  end while
  $\phi_0 \leftarrow \theta$
Output: the meta-parameters ϕ_0

Algorithm 2 Implicit Neural Representation Learning for Target Sample

Input: $D^* = (t_{ij}, y_{ij})_{j=1}^{J^*}$: the sparse observations for the target task
Input: α : step size hyperparameters
  initialize $\phi \leftarrow \phi_0$
  while not done **do**
    Evaluate $\nabla_\phi \mathcal{L} \left(F_\phi\right)$ using support set $D^* = (t_j^*, y_j^*)_{j=1}^{J^*}$
    Update parameters with gradient descent: $\phi = \phi - \alpha \nabla_\phi \mathcal{L} \left(F_\phi\right)$
  end while
  $\phi^* \leftarrow \phi$
Output: ϕ^*: the parameters of INR for the target model

In our approach, we view meta-learning not merely as an efficient learning method but as a means to learn commonalities among a large number of tasks. Leveraging this property, the metaINR $\hat{y}_i(t) = F_{\phi_i^*}(t)$ implicitly contain the information of the whole datasets. Consequently, it provides a reliable estimation for sparse time series data.

MetaINR versus other learning-based INR for sparse data

4 Experiments

We evaluate our method on the synthetic data, with benchmark estimations provided by local polynomial regression and the traditional PACE method [TODO]. Our results clearly demonstrate that MetaINR significantly outperforms the conventional baseline. Moreover, we extended our analysis to a real-world medical dataset to validate the robustness and applicability of our approach in practical scenarios.

4.1 Synthetic data

[IDEA: synthetic data generated by DE + evaluation principle]

Data generating process Our ground truth of our synthetic data distribution is given by:

$$y(t) = Asin(t) + Bsin(2t), \quad t \in [0, 10],$$

where A and B are independent and follows the uniform distribution

$$A \sim Uniform[0, 1], \quad B \sim Uniform[0, 0.5].$$

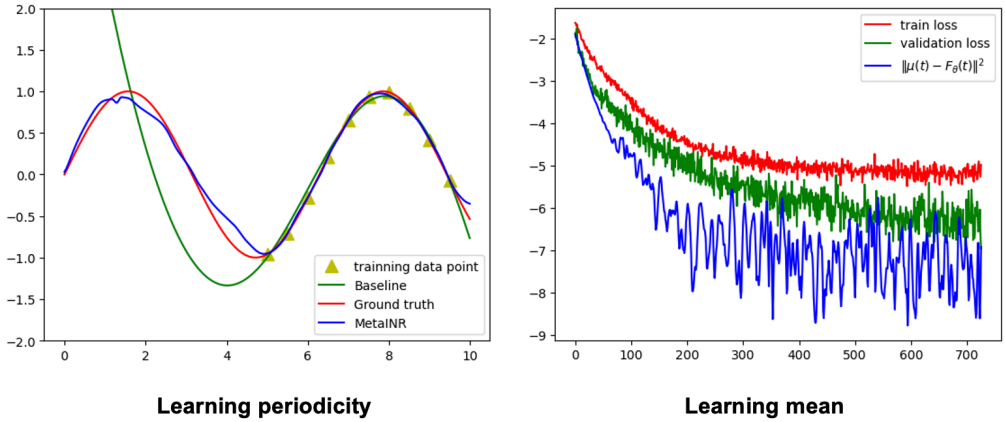

Figure 1: Learning commonalities

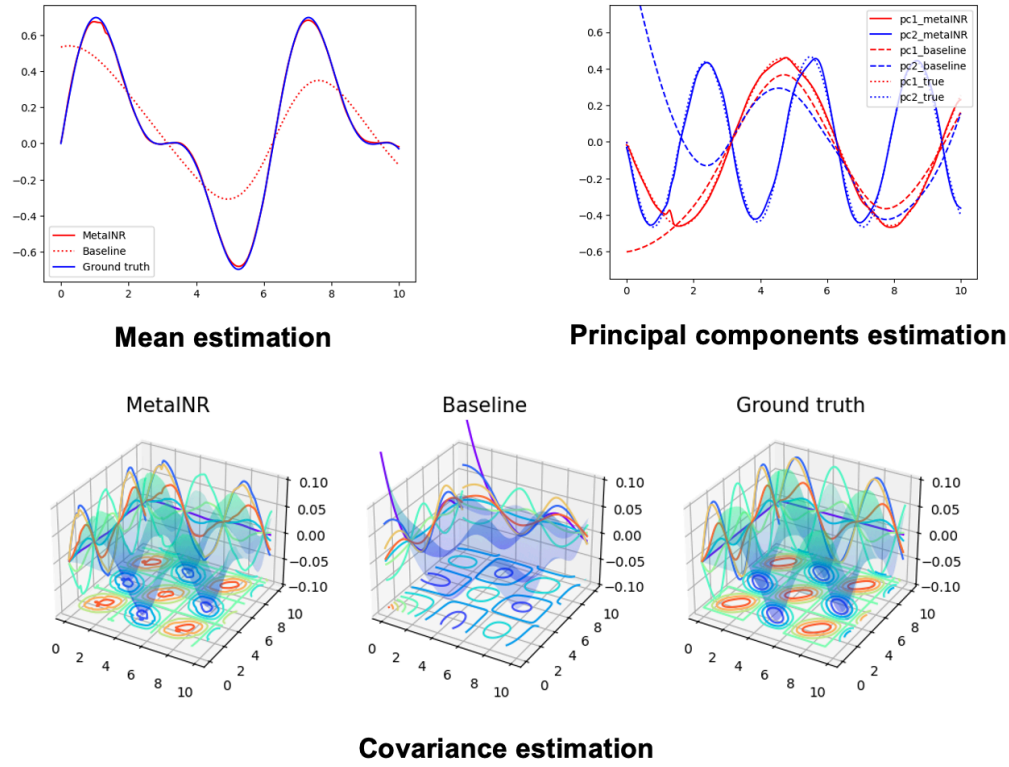

Figure 2: Estimation for synthetic data

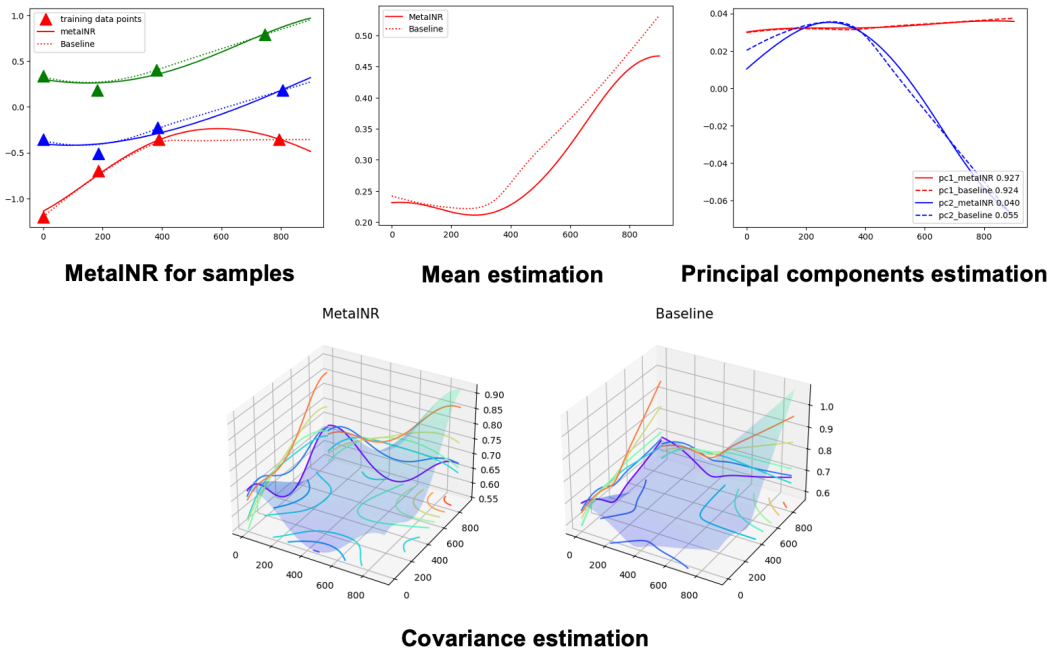

Figure 3: Estimation for real-world data

We randomly draw $n = 100$ sample tasks $\{y_i(t)\}_{i=1}^n$ from this distribution. For each sample task, $J = 20$ observations randomly chosen in irregular time points. The overall dataset used for meta-learning comprises these observations.

$$D = \{(t_{ij}, y_{ij})_{j=1}^J\}_{i=1}^n$$

Meta-learning the commonalities of time series When conducting meta-learning on this synthetic dataset, we indeed observed the capability of meta-learning to capture commonalities among a series of similar time-series data. As shown in Figure 1a, we found that when providing observations solely for the latter segment ($t \in [5, 10]$) of a particular sample, meta-learning could extract information from data of other samples, learning the periodicity inherent in this distribution. In contrast, local polynomial regression relies solely on the data of an individual sample for estimation, resulting in less accurate predictions for the first half ($t \in [0, 5]$) of the time series. In addition, we discovered that the meta-model inherently contains information about the mean. By directly plugging the initial values learned by MAML into the SIREN model to construct our meta-model for further learning, we observed a notable proximity between the meta-model and the means of these samples. As demonstrated in Figure 1b, the meta-learning process is accompanied by the meta-model gradually converging towards the mean. Aside from these two examples, [2] illustrates that MAML accelerates learning through feature reuse. This also clarifies why the meta-model encompasses various features of the dataset. Consequently, employing MetaINR for time series reconstruction based on sparse observations proves to be more reliable than local polynomial regression.

Estimation of mean, covariance and principal components

Based on MetaINR for each sample, we estimated the mean function, covariance kernel, and principal components of this synthetic dataset. The results are demonstrated in Figure 2. We observed that the estimators based on MetaINR for all three metrics significantly outperformed the benchmark. Particularly at the boundaries of the data, where t approaches 0 or 10, the baseline estimators often deviated substantially from the true values, while the estimators based on MetaINR remained relatively reliable.

4.2 Real-world data

Data description In real-world scenarios, we apply MetaINR to the longitudinal data on primary biliary cirrhosis (PBC). The data resulted from a Mayo Clinic trial that was conducted in 1974 to 1984. They are available at http://lib.stat.cmu.edu/datasets/pbc and have been described in Fleming & Harrington (1991) and Murtaugh et al. (1994). The data contain various sparsely and irregularly sampled covariates, as well as the survival or censoring time for each of 312 patients. Among these medical measurements, serum bilirubin concentration is known to be elevated in the presence of chronic liver cirrhosis, such as PBC. We extracted data from the dataset for the initial 910 days, analyzing bilirubin measurements (in mg/dl) for different patients during the pre-onset phase. The goal was to characterize the pattern of this measurement over time through estimates of mean function, covariance kernel and principal components. In practice, we applied a logarithmic transformation to the bilirubin measurements and removed data for patients with a survival time less than 910 days. A total of 260 patients in the study satisfied these criteria and only 2.9 observations per sample on average.

Estimation of mean, covariance and principal components Figure 3 illustrates the estimation results of MetaINR on the real-world medical sparse functional dataset mentioned above. We observe that despite the minimal number of observations per sample, MetaINR can effectively recover the sample function. Regarding the estimation of statistical quantities, MetaINR demonstrates similar performance to the baseline in this specific real dataset. From the estimation results, we draw the following conclusions: Over the initial 910 days of observation, patients' serum bilirubin concentration initially experiences a slight decrease, followed by a sharp increase around 400 days (mean function). Apart from differences in "baseline values" which remain invariant with time (PC1), significant divergence in serum bilirubin concentration among patients emerges around 400 days (PC2).

5 Conclusion and future work

In this paper, we have shown a method named MetaINR utilizing meta-learning to analyze sparse time series data. MetaINR enables the estimation of functional form samples with very few observation points by leveraging information from the entire dataset through meta-learning. The application of MetaINR makes functional data analysis (FDA) methods, which are typically used in dense datasets, feasible for sparse datasets. Therefore, MetaINR provides a novel tool for further analyzing sparse time series data.

In future research, we aim to extend the application of MetaINR to other functional data analysis methods that were initially designed for dense datasets, such as Functional Partial Least Squares Regression (FPLS), functional regression, registration and more. We can also explore other algorithms of meta-learning, such as SNAIL, and compare the performances between them.

6 Appendix

6.1 Traditional FDA method for sparse functional data: PACE

6.2 Brief introduciton to SIREN

6.3 Experiments on other synthetic data

Data and code availability

PBC data used in this paper is available at `http://lib.stat.cmu.edu/datasets/pbc` , and it also can be found in a R package called "survival". All the experimental code in this paper is available at `https://github.com/cbfcbf/code_metaINR`.

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