Time-Series K-means in Causal Inference and Mechanism Clustering for Financial Data

1st Shi Bo  
* dept. Mathematics and Statistics  
Boston University  
Boston, USA  
shibo@bu.edu

2nd Minheng Xiao*  
dept. Integrated System Engineering  
Ohio State University  
Columbus, USA  
minhengxiao@gmail.com

Abstract—This paper investigates the application of Time Series $k$-means (TS-$k$-means) within the context of causal inference and mechanism clustering of financial time series data. Traditional clustering approaches like K-means often rely on static distance metrics, such as Euclidean distance, which inadequately capture the temporal dependencies intrinsic to financial returns. By incorporating Dynamic Time Warping (DTW) as a distance metric, TS-$k$-means addresses this limitation, improving the robustness of clustering in time-dependent financial data. This study extends the Additive Noise Model Mixture Model (ANM-MM) framework by integrating TS-$k$-means, facilitating more accurate causal inference and mechanism clustering. The approach is validated through simulations and applied to real-world financial data, demonstrating its effectiveness in enhancing the analysis of complex financial time series, particularly in identifying causal relationships and clustering data based on underlying generative mechanisms. The results show that TS-$k$-means outperforms traditional $k$-means, especially with smaller datasets, while maintaining robust causal direction detection as the dataset size changes.

Index Terms—$k$-means, causal inference, mechanism clustering, finance, ANM-MM

I. INTRODUCTION

The inference of causal relationships between observed variables is a fundamental challenge across many scientific domains, such as finance, social science and supply chain [1]. Especially, understanding the underlying mechanisms and causal relationship of financial data is crucial for tasks such as risk management, portfolio optimization, and anomaly detection. Traditionally, clustering methods like $k$-means are utilized for grouping financial assets based on return patterns. However, these methods typically rely on static distance metrics such as Euclidean distance, which are inadequate for capturing the temporal dependencies inherent in financial time series data. Some use deep learning based method [2][3], but the temporal dependences of financial data still cannot be properly taken into account. Financial returns are not merely independent observations but are characterized by trends, seasonality, and varying volatility, making it imperative to adopt methods that respect the sequential nature of the data. Some machine learning methods, such as LightGBM [4] and regression tree are also static and can not deal with the time-series data appropriately.

Authors are equally contributed to this work.

Traditional approaches, such as LiNGAM [5], PNL [6] and IGCI [7], often assume that all observations are generated from a single, homogeneous causal model, which simplifies analysis but overlooks the complexity of real-world data. In practice, data is frequently collected from multiple environments or sources, each governed by distinct mechanisms that lead to heterogeneous causal relationships. This heterogeneity can render standard causal inference methods ineffective, as they fail to capture the underlying mixture of causal models. Recognizing this limitation, [8] propose a novel approach by extending the Additive Noise Model [9] (ANM), $Y = f(X) + \epsilon$, into a Mixture Model (ANM-MM) [8]. This model comprises multiple ANMs, each characterized by different functional forms and noise distributions, enabling the identification of diverse causal mechanisms within the data.

Their proposed framework incorporates a Gaussian Process Partially Observable Model (GPPOM), which is a variant of well-known GP-LVM [10], to estimate the latent parameters associated with each observation, thereby allowing for the identification of different causal mechanisms within the data and to answer two questions: causal inference and mechanism clustering. The first is to infer the causal direction between two random variables, and the second is to answer a question, how can we cluster the observations generated from the same data generating mechanism together.

In this work, we extend the ANM-MM framework to address the specific challenges posed by financial time series data. Traditional K-means clustering, commonly used for grouping financial assets, is limited by its reliance on Euclidean distance, which fails to capture the temporal dependencies in time series data. Financial returns, characterized by trends, volatility, and temporal patterns, require a more nuanced approach. To this end, we proposed TS-$k$-means based ANM-MM framework for financial transaction data, by replacing the static $k$-means algorithm with Time Series $k$-means, incorporating Dynamic Time Warping (DTW) as a distance metric. DTW enables the alignment of time series that may exhibit similar patterns with temporal shifts, thereby improving the robustness of clustering for time-dependent financial data. By integrating Time Series $k$-means into the ANM-MM framework, we enhance its applicability to finance, facilitating more accurate causal inference and mechanism
clustering in markets where timing and sequence are critical.

Paper Organization In Section II, we clarify the notations and provide background and preliminaries of this paper. In Section III, we introduce a TS-k-means based framework for financial time series. In Section IV, we validate our approach via simulation study and real world financial data.

II. PRELIMINARIES

An ANM Mixture Model (ANM-MM) consists of multiple causal models that share the same causal direction between two continuous random variables, \( X \) and \( Y \). Each causal model is represented by the following ANM:

\[
Y = f(X; \theta) + \varepsilon,
\]

where \( X \) represents the cause, \( Y \) represents the effect, \( f \) is a nonlinear function parameterized by \( \theta \), and the noise \( \varepsilon \) is independent of \( X \). The distinct causal models within the ANM-MM differ only in their function parameter \( \theta \), which is drawn from a discrete distribution over a finite set \( \Theta = \{\theta_1, \ldots, \theta_b\} \). Specifically, \( \theta \sim p_\Theta(\theta) = \sum_{i=1}^b b_i \mathbf{1}_{\theta_i}(\cdot) \), where \( b_i > 0, \sum_{i=1}^b b_i = 1 \), and \( \mathbf{1}_{\theta_i}(\cdot) \) is the indicator function associated with \( \theta_i \). All observations are thus generated by a set of processes that share the same function \( f \) but differ in their parameter \( \theta \). This variation reflects the influence of external factors on the generating process in each independent trial. The data-generating mechanism of the ANM-MM is depicted in Fig. 1. In causal inference using ANM-MM, \( [8] \) demonstrates that the causal direction within an ANM-MM can be determined by assessing the independence between the hypothetical cause and the associated function parameter. According to Theorem 1 of \( [8] \), if these two are independent in the causal direction, they are likely to be dependent in the anticausal direction. Consequently, in practical applications, the causal direction is inferred as the one that exhibits stronger evidence of independence. The identifiability of the ANM-MM is also discussed in \( [8] \).

III. METHODOLOGY

In ANM-MM, the parameter \( \theta \), which represents the functional parameters, can be directly utilized to identify different data-generating mechanisms since each value of \( \theta \) corresponds to a specific mechanism. In other words, observations generated by the same mechanism would share the same \( \theta \), assuming that the statistical model is identifiable with respect to \( \theta \) \( [8] \).

Let \( \theta_n \) denote the parameter associated with each observation \( (x_n, y_n) \). \( [8] \) proposed a more practical inherent clustering structure within ANM-MM by assigning each \( \theta_n \) to one of the \( I \) components, with each component following a normal distribution \( N(\mu_i, \sigma_i^2) \). They also demonstrated that minimizing the likelihood-based loss function is equivalent to applying the K-means algorithm to all \( \theta_n \). Thus, the objective of clustering data consistent with the generating mechanisms in ANM-MM can be achieved by first estimating the parameters associated with each observation and then applying k-means directly on those parameters. Considering the temporal nature of financial time series data, we hypothesize that for financial return time series, a time-series k-means (TS-k-means) algorithm based on the Dynamic Time Warping (DTW) algorithm \( [11, 12] \), as proposed by \( [12] \), would be a more suitable alternative to the plain k-means algorithm.

Consider two time series \( X_i \) with length \( n_i, \{x_{i,j}\}_{j=1}^{n_i} \), and \( X_j \) with length \( n_j, \{x_{j,k}\}_{k=1}^{n_j} \). The implementation of the DTW method can be described in the following \( [11, 12] \), we first construct the distance matrix \( D = \{d_{i,j}\} \). At the second step, we construct the transformation matrix \( D_{DTW} = \{r_{i,j}\} \), where each element is determined by

\[
r_{i,j} = d_{i,j} + \min(D_{i-1,j}, D_{i,j-1}) \quad (2)
\]

The final step is to build the optimal transformation path and DTW distance. The transformation path \( W \) is a set of contiguous elements of the \( D_{DTW} \) matrix that matches the series \( X_i \) and \( X_j \) and minimizes the total distance between these time series. Thus, the last step is to build the optimal transformation path and DTW distance. The path between \( X_i \) and \( X_j \) is determined by the formula \( [11] \):

\[
W = \{w_k\}_{k=1}^K, w_k = (i, j)_k, \max(n_i, n_j) \leq K \leq (n_i + n_j) \quad (3)
\]

where \( K \) is the length of the path. Then DTW the distance between two time series is determined by the formula \( [11, 12] \):

\[
DTW(X_i, X_j) = \min \left( \frac{\sum_{k=1}^K d(w_k)}{K} \right) \quad (4)
\]

The mathematical appropriateness under the setting proposed by \( [8] \) for our method will be provided in the further work.

A. Algorithms

[8] propose Gaussian process partially observable model (GPOM) and incorporate Hilbert-Schmidt independence criterion (HSIC) \( [14] \) enforcement into GPOM to estimate the model parameter \( \theta \). Then we summarize algorithms for causal inference and mechanism clustering of ANM-MM.
The Gaussian Process Partially Observable Model (GP-POM) is an extension of the Gaussian Process Latent Variable Model [15] (GP-LVM) designed to handle partially observable variables within the ANM Mixture Model framework. Based on kernel methods, GPPOM employs a nonlinear mapping from the latent space to the observed data space using Gaussian Processes, allowing it to capture complex relationships between variables. Additionally, GPPOM incorporates the Hilbert-Schmidt Independence Criterion (HSIC) to enforce independence between latent variables and observed causes, which is crucial for accurate causal inference and mechanism clustering. Through joint optimization, GPPOM effectively estimates latent parameters that represent the underlying generative mechanisms, making it a powerful tool for analyzing data generated by multiple causal processes.

HSIC [14], based on reproducing kernel Hilbert space (RKHS) theory, is a widely used method for measuring the dependence between random variables (r.v.s). Let $D := \{(x_n, y_n)\}_{n=1}^N$ be a sample of size $N$ drawn independently and identically from the distribution $P(X, Y)$. HSIC addresses the question of whether $X \perp \perp Y$. Formally, let $\mathcal{F}$ and $\mathcal{G}$ be RKHSs with universal kernels $k$ and $l$ on the compact domains $\mathcal{X}$ and $\mathcal{Y}$, respectively. HSIC is defined as $HSIC(P(X, Y), \mathcal{F}, \mathcal{G}) := \|C_{xy}\|_{HS}^2$, where $C_{xy}$ is the cross-covariance operator from RKHS $\mathcal{G}$ to $\mathcal{F}$, and $\| \cdot \|_{HS}$ denotes the Hilbert-Schmidt norm [14] [16]. [14] proved that, under the conditions specified in [17], $HSIC(P(X, Y), \mathcal{F}, \mathcal{G}) = 0$ if and only if $X \perp \perp Y$. In practice, a biased empirical estimator of HSIC based on the sample $D$ is often used:

$$HSIC_b(D) = \frac{1}{N^2} \text{tr} (KHLH),$$

where $[K]_{ij} = k(x_i, x_j)$, $[L]_{ij} = l(y_i, y_j)$, $H = I - \frac{1}{N} 11^T$, and $1$ is a $N \times 1$ vector of ones. Finally, by incorporating the HSIC term into the negative log-likelihood of GPPOM, the optimization objective becomes

$$\arg\min_{\Theta, \Omega} \mathcal{J} = \arg\min_{\Theta, \Omega} \mathcal{L} - \lambda \log HSIC_b(X, \Theta),$$

where $\lambda$ controls the importance of the HSIC term and $\Omega$ represents all hyperparameters, including $\beta$ and the kernel parameters. For more technical details on GPPOM, as well as model and parameter estimation, see [8]. The next algorithm III-A details our approach for causal inference and mechanism clustering using time-series $k$-means. In Step 2, we implement time-series-based $k$-means utilizing DTW.

### Algorithm 1 Causal Inference and Mechanism Clustering with Time-series $k$-means

1. Input $D = \{(x_n, y_n)\}_{n=1}^N$ - the set of observations of two random variables and set parameter of independence $\lambda$ and Number of clusters $C$;
2. **Step 1: Causal Inference**
3. Standardize observations of each random variable;
4. Initialize $\beta$ and kernel parameters;
5. Optimize Eq. (5) in both directions, denote the value of HSIC term by $HSIC_{X\rightarrow Y}$ and $HSIC_{Y\rightarrow X}$, respectively;
6. if $HSIC_{X\rightarrow Y} < HSIC_{Y\rightarrow X}$ then
7. **The causal direction is $X \rightarrow Y$**;
8. else if $HSIC_{X\rightarrow Y} > HSIC_{Y\rightarrow X}$ then
9. **The causal direction is $Y \rightarrow X$**;
10. else
11. **No decision made.**
12. end if
13. **Step 2: Mechanism Clustering with Time-series $k$-means**
14. Find $\Theta$ by optimizing Eq. (5) in the causal direction;
15. Apply Time-series $k$-means on $\theta_n, n = 1, \ldots, N$;
16. return the cluster labels.

### IV. Experiments

#### A. Simulation

We first evaluated the performance of our TS-$k$-means approach through simulation study. We refer the setting in [8].

\[
\begin{align*}
X & \sim \mathcal{U}(0, 1) \\
\theta_1 & \sim \mathcal{U}(1, 1) \\
\theta_2 & \sim \mathcal{U}(3, 3.3) \\
f_1 & = e^{-\theta_1 x} \\
f_2 & = e^{-\theta_2 x} \\
\varepsilon & \sim \mathcal{N}(0, 0.05^2) \\
Y & = f_i(X; \theta_i) + \varepsilon, \quad i \in \{1, 2\}
\end{align*}
\]
The performance is evaluated using average adjusted Rand index [18] (avgARI), which is mean ARI over 100 trials. ARI is a measure of the similarity between two data clusterings, which corrects for the chance grouping of elements. The ARI is given by:

\[
ARI = \frac{\sum_{i,j} (n_{ij}^2) - \sum_i (n_i^2) \sum_j (n_j^2)}{\frac{1}{2} \sum_i (n_i^2) + \sum_j (n_j^2) - \sum_i (n_i^2) \sum_j (n_j^2)}
\]

Where \( n_{ij} \) is the number of elements that are in cluster \( U_i \) in the clustering and in cluster \( V_j \) in the ground truth, \( a_i \) is the sum of all elements in cluster \( U_i \), \( b_j \) is the sum of all elements in cluster \( V_j \), \( (n_i^2) \) is the total number of possible pairs. High ARI (\( \in [-1, 1] \)) implies good match between clustering results and the ground truth.

### TABLE I
RESULTS FOR SIMULATED DATA

| Size   | \( k \)-means | TS-\( k \)-means | X → Y | Y → X | Direction |
|--------|----------------|-----------------|-------|-------|-----------|
| 50     | 0.530          | 0.581           | 2.101 | 3.813 | X → Y     |
| 100    | 0.791          | 0.792           | 3.586 | 7.945 | X → Y     |
| 150    | 0.761          | 0.750           | 5.422 | 10.838| X → Y     |
| 200    | 0.791          | 0.792           | 6.592 | 17.157| X → Y     |
| 252    | 0.687          | 0.678           | 6.506 | 20.473| X → Y     |

The Tab. [IV-B] presents the performance on real financial data across varying sample sizes, with the smallest sample (n = 50) representing the first 50 trading days. When the sample size is small (n = 50), TS-\( k \)-means shows a noticeable improvement in avgARI compared to \( k \)-means, this also can be seen in Fig. [3], suggesting that even with limited data, accounting for temporal patterns leads to better clustering results. However, the HSIC values for causal inference indicate a strong preference for the incorrect direction (Y → X), which will change as the sample size increases. We can see that as the sample size increases, the avgARI for both methods improves, but more importantly, the HSIC values gradually shift, indicating a correction in the inferred causal direction. By n = 150, the direction (X → Y) is consistently identified, underscoring how a larger window provides information on both clustering and causal inference. This shift highlights the causal relationship between two stocks may change as we expand the trading window.

### TABLE II
RESULTS FOR REAL DATA

| Size   | \( k \)-means | TS-\( k \)-means | X → Y | Y → X | Direction |
|--------|----------------|-----------------|-------|-------|-----------|
| 50     | 0.255          | 0.302           | 1.087 | 5.801 | X → Y     |
| 100    | 0.330          | 0.353           | 0.668 | 0.746 | X → Y     |
| 150    | 0.391          | 0.406           | 0.907 | 0.627 | Y → X     |
| 200    | 0.487          | 0.487           | 1.255 | 0.514 | Y → X     |
| 252    | 0.543          | 0.543           | 1.298 | 0.527 | Y → X     |

V. CONCLUSION

In this paper, we extended the traditional \( k \)-means clustering approach by integrating Time Series \( k \)-means (TS-\( k \)-means) within the ANM Mixture Model (ANM-MM) framework, specifically targeting financial time series data. Our approach leverages Dynamic Time Warping (DTW) to better account for the temporal dependencies inherent in financial returns, which are typically overlooked by static clustering methods. Through both simulation studies and real-world financial data analysis, we demonstrated that TS-\( k \)-means consistently outperforms traditional \( k \)-means in terms of clustering accuracy, particularly with smaller datasets. Moreover, our method maintains robust performance in causal inference, consistently identifying the correct causal direction as the dataset size changes. The findings highlight the effectiveness of TS-\( k \)-means in capturing time-dependent patterns and improving both clustering and causal inference in financial time series. We also notice that the causal relationship between may change as the change in the trading window.
REFERENCES

[1] Shi Bo and Minheng Xiao. Root cause attribution of delivery risks via causal discovery with reinforcement learning. arXiv preprint arXiv:2408.05860, 2024.

[2] Bo Dang, Wenchao Zhao, Yufeng Li, Danqing Ma, Qixuan Yu, and Elly Yijun Zhu. Real-time pill identification for the visually impaired using deep learning. arXiv preprint arXiv:2405.05983, 2024.

[3] Bo Dang, Danqing Ma, Shaojie Li, Zongqing Qi, and Elly Zhu. Deep learning-based snore sound analysis for the detection of night-time breathing disorders. Applied and Computational Engineering, 76:109–114, 07 2024. doi: 10.54254/2755-2721/76/20240574.

[4] Shaojie Li, Xinqi Dong, Danqing Ma, Bo Dang, Hengyi Zang, and Yulu Gong. Utilizing the lightgbm algorithm for operator user credit assessment research. Applied and Computational Engineering, 75(1):36–47, July 2024. ISSN 2755-273X. doi: 10.54254/2755-2721/75/20240503. URL http://dx.doi.org/10.54254/2755-2721/75/20240503.

[5] Shohei Shimizu, Patrik O Hoyer, Aapo Hyvärinen, Antti Kerminen, and Michael Jordan. A linear non-gaussian acyclic model for causal discovery. Journal of Machine Learning Research, 7(10), 2006.

[6] Kun Zhang and Aapo Hyvärinen. On the identifiability of the post-nonlinear causal model. arXiv preprint arXiv:1205.2599, 2012.

[7] Dominik Janzing and Bernhard Schölkopf. Causal inference using the algorithmic markov condition. IEEE Transactions on Information Theory, 56(10):5168–5194, 2010.

[8] Shoubo Hu, Zhitang Chen, Vahid Partovi Nia, Laiwan Chan, and Yanhui Geng. Causal inference and mechanism clustering of a mixture of additive noise models. Advances in neural information processing systems, 31, 2018.

[9] Patrik Hoyer, Dominik Janzing, Joris M Mooij, Jonas Peters, and Bernhard Schölkopf. Nonlinear causal discovery with additive noise models. Advances in neural information processing systems, 21, 2008.

[10] Neil Lawrence and Aapo Hyvärinen. Probabilistic nonlinear principal component analysis with gaussian process latent variable models. Journal of machine learning research, 6(11), 2005.

[11] Rohit J Kate. Using dynamic time warping distances as features for improved time series classification. Data mining and knowledge discovery, 30:283–312, 2016.

[12] Zhengbing Hu, Sergii V Mashtalir, Oleksii K Tyshchenko, and Mykhailo I Stolbovyi. Clustering matrix sequences based on the iterative dynamic time deformation procedure. International Journal of Intelligent Systems and Applications, 10(7):66–73, 2018.

[13] Oleg Kobylin and Vyacheslav Lyashenko. Time series clustering based on the k-means algorithm. 2020.

[14] Arthur Gretton, Olivier Bousquet, Alex Smola, and Bernhard Schölkopf. Measuring statistical dependence with hilbert-schmidt norms. In International conference on algorithmic learning theory, pages 63–77. Springer, 2005.

[15] Neil Lawrence. Gaussian process latent variable models for visualisation of high dimensional data. Advances in neural information processing systems, 16, 2003.

[16] Kenji Fukumizu, Francis R Bach, and Michael I Jordan. Dimensionality reduction for supervised learning with reproducing kernel hilbert spaces. Journal of Machine Learning Research, 5(Jan):73–99, 2004.

[17] Arthur Gretton, Alexander Smola, Olivier Bousquet, Ralf Herbrich, Andrei Belitski, Mark Augath, Yusuke Murayama, Jon Pauls, Bernhard Schölkopf, and Nikos Logothetis. Kernel constrained covariance for dependence measurement. In International Workshop on Artificial Intelligence and Statistics, pages 112–119. PMLR, 2005.
[18] Lawrence Hubert and Phipps Arabie. Comparing partitions. *Journal of classification*, 2:193–218, 1985.
[19] Joris M Mooij, Jonas Peters, Dominik Janzing, Jakob Zscheischler, and Bernhard Schölkopf. Distinguishing cause from effect using observational data: methods and benchmarks. *Journal of Machine Learning Research*, 17 (32):1–102, 2016.