Multiscale Causal Structure Learning

Abstract

Causal structure learning methods are vital for unveiling causal relationships embedded into observed data. However, the state of the art suffers a major limitation: *it assumes that causal interactions occur only at the frequency at which data is observed.* To address this limitation, this paper proposes a method that allows structural learning of linear causal relationships occurring at different time scales. Specifically, we explicitly take into account instantaneous and lagged inter-relations between multiple time series, represented at different scales, hinging on wavelet transform. We cast the problem as the learning of a *multiscale causal graph* having *sparse* structure and *dagness* constraints, enforcing causality through directed and acyclic topology. To solve the resulting (non-convex) formulation, we propose an algorithm termed MS-CASTLE, which exhibits consistent performance across different noise distributions and wavelet choices. We also propose a single-scale version of our algorithm, SS-CASTLE, which outperforms existing methods in computational efficiency, performance, and robustness on synthetic data. Finally, we apply the proposed approach to learn the multiscale causal structure of the risk of 15 global equity markets, during covid-19 pandemic, illustrating the importance of multiscale analysis to reveal useful interactions at different time resolutions. Financial investors can leverage our approach to manage risk within equity portfolios from a causal perspective, tailored to their investment horizon.

1 Introduction

The study of causal relationships plays a fundamental role in our understanding of complex systems. However, learning causal relationships is a challenging task, and often is not even possible to directly act on the systems of interest (e.g., social networks) because of ethics, feasibility, or cost issues. Thus, the ability to unravel causal structures from the observed data, also known as *causal structure learning*, is an attractive technology that has received growing attention in the last years, also thanks to the ever-increasing volume of available data, see e.g., (Pearl, 2009; Peters et al., 2017b; Glymour et al., 2019; Schölkopf et al., 2021). In the literature, several works hinged on directed acyclic graphs (DAGs) to represent causal dependencies (i.e., directed edges) between the constituents (e.g., nodes) of the considered system (Vowels et al., 2022). Indeed, the acyclicity requirement represents a necessary condition in order to set causes apart from effects; a result that cannot be accomplished in the presence of feedback loops among the nodes. In case the nodes of the DAG are associated with time series observations, the dependencies represented by the DAG refer to causal interactions occurring between the values of the time series within the same timestamp and across different time stamps. The formers are called *instantaneous*, whereas the latters, since we can only observe causal interactions coming from the past, are named *lagged*.

Related works. Causal structure learning algorithms can be classified in accordance with the approach used to infer the associated DAG. In particular, we can identify three main different classes: (i) *constraint-based approaches*, which run conditional independence tests to validate the presence of an edge between two variables (Spirtes et al., 2000; Huang et al., 2020); (ii) *score-based methods*, which measure the goodness of fit of graphs according to a given criterion and then use search procedures to explore the solution space (Heckerman et al., 1995; Chickering, 2002; Huang et al., 2018); (iii) *functional methods*, which model a variable in terms of a function of its parents (Shimizu et al., 2006; Hoyer et al., 2008; Hyvärinen et al., 2010; Peters et al., 2014; Bühlmann et al., 2014). Furthermore, a recent important contribution came by

reformulating the problem of learning a DAG using a suitable continuous non-convex penalty (Zheng et al., 2018; 2020). This enabled the usage of gradient-based methods (Yu et al., 2019; Lachapelle et al., 2020; Ng et al., 2020) and reinforcement learning (Zhu et al., 2020) in causal discovery problems.

Whenever we deal with causal inference for time series analysis, we need to take into account time ordering as well. Considering linear models, this leads to the formulation of the *structural vector autoregressive model* (SVARM) (Kilian & Lütkepohl, 2017), which can be thought of a combination of a *structural equation model* (SEM) (Peters et al., 2017a) and a *vector autoregressive model* (VAR) (Sims, 1980). To estimate the SVARM parameters, a stream of research assumes the endogenous noise to be non-normally distributed (Hyvärinen et al., 2010; Moneta et al., 2013). This allows us to apply *independent component analysis* (ICA) to infer the causal structure from observations (Hyvarinen, 1999). Then, leveraging non-convex optimization, DYNOTEARS showed promising results in the task of causal structure learning for time series (Pamfil et al., 2020). From the optimization point of view, the *alternating direction method of multipliers* (ADMM) (Boyd et al., 2011) is also exploited in several works for causal structural learning, see, e.g., (Ng & Zhang, 2022; Yang et al., 2022; Harada & Fujisawa, 2021). As detailed in Section 3, also the method proposed in this paper will hinge on ADMM but, differently from Ng & Zhang (2022) and Yang et al. (2022), we leverage a modified ADMM algorithm that exploits a linearization of the non-convex dagness function introduced by Zheng et al. (2018). In Harada & Fujisawa (2021), ADMM applies to a linearly-constrained problem having a different objective function. Also, differently from our method, the approach in Harada & Fujisawa (2021) is viable only if the latent noise is assumed to be non-Gaussian.

Regardless of the assumed causal model, all previous works suffer a major limit, that is, they only consider instantaneous and lagged interactions at the time resolution corresponding to the observational task. However, the introduction of multiscale analysis is of paramount importance since it represents a key feature of complex systems, as shown in Calvet & Fisher (2001); Kwapień & Drożdż (2012). In particular, wavelet analysis, together with network analysis, has been already employed in the study of financial risk contagion (Loh, 2013; Khalfaoui et al., 2015; Wang et al., 2017). More recently, the integration of machine learning methods and multiscale representations has been proven to provide significant advancements in biological and behavioral sciences, as reported in Alber et al. (2019) and Peng et al. (2021). Consider for example fMRI data regarding different brain regions of interest (ROIs) collected at timestamps $t \cdot \Delta t$, with Δt being the time interval between two consecutive samples. The aforementioned limit translates into the inability of studying causal interactions between ROIs over time resolutions coarser than Δt, while it is known that the connectivity between ROIs varies over different time scales, also depending on the state of the brain (Jacobs et al., 2007; Ciuciu et al., 2014; Ide et al., 2017).

Other examples can be found in other application domains (Besserve et al., 2010; Gong et al., 2015; Runge et al., 2019), and in general there is no prior knowledge about the time scales at which important causal relations occur. Recently, D'Acunto et al. (2022) proposed a probabilistic generative model and an inference method for multiscale DAGs. In contrast to that work, our methodology (i) relies on wavelet transform, generalizing the SVAR model to the time-frequency domain, (ii) enables learning of multiscale relationships across different time lags while making no assumptions on the causal ordering at each scale, and (iii) has a lower computational cost, thus allowing analysis of networks with a larger number of nodes. For these reasons, we consider the method in (D'Acunto et al., 2022) incomparable to our algorithm. Overall, the combination of multiscale representation with causal learning is still an open problem and this motivates the proposed work.

Contributions. In this paper, we overcome the limit of previous approaches by proposing a *linear causal inference algorithm based on a multiscale representation*, able to capture the most relevant causal dependencies across multiple time scales and time lags. Specifically, we start formulating an optimization problem aimed at learning a multiscale causal graph from data, while taking into account sparsity and enforcing causality through directed and acyclic topology. Then, as reported in Section 3, we exploit a customized version of linearized ADMM (useful to copy with the non-convexity of the problem at hand), thus deriving the proposed *Multiscale-Causal Structure Learning* (MS-CASTLE) algorithm. As a particular case, MS-CASTLE includes a single time scale version, which we term *Single-scale-Causal Structure Learning* (SS-CASTLE), to learn causal connections at the frequency of observed data.

To summarize, the paper has three main contributions:

- **Multiscale structure learning.** Firstly, we propose a multiscale causal inference algorithm that allows the extraction of causal links at different time scales, without requiring any prior knowledge of the scale where causal relations are most effective. We evaluate the performance of MS-CASTLE from synthetic data generated according to a multiscale causal structure. The results of our empirical assessment, illustrated in Section 4.3, suggest that MS-CASTLE is suitable for both Gaussian and non-Gaussian settings, and that is robust to different choices of the wavelet family used to decompose the input time series.

- **Application to financial markets.** Secondly, we showcase the application of our proposals on real-world financial time series in Section 5. Specifically, we apply MS-CASTLE to learn the causal dynamics of risk contagion among 15 global equity markets during covid-19 pandemic, from January 2, 2020 to April 30, 2021, and we compare the resulting graphs with those retrieved by single-scale causal learning methods. Our analysis shows that MS-CASTLE provides richer information regarding the causal structure of the system that cannot be understood by looking only at the estimated single-scale causal graph. In particular, our findings suggest that: i) causal connections are characterized by positive weights and are denser at mid-term time resolution (scales 3 and 4, i.e., 8-16 and 16-32 days, respectively); ii) the strongest connections are lagged and they appear at scales 3 and 4; iii) the markets injecting the majority of risk into the network are Brazil, Canada and Italy. Further discussions concerning the obtained results and the richness of information gained through the multiscale causal analysis are given in Section 5.4. Our analysis of financial time series provides novel results at both methodological as well as application levels with respect to the stream of research known as *Econophysics* (Mantegna & Stanley, 1999). At the methodological level, we propose a multiscale machine learning causal model that, differently from existing work (Billio et al., 2012), allows us to analyse both instantaneous and lagged causal interactions at distinct time scales. At the application level, we apply MS-CASTLE to learn the causal dynamics of risk contagion among 15 global equity markets during covid-19 pandemic, rather than focusing on financial institutions.

- **Single-scale structure learning.** Finally, we compare the single-scale version of our algorithm, i.e., SS-CASTLE, with several baselines (Pamfil et al., 2020; Hyvärinen et al., 2010; Hyvarinen, 1999; Shimizu et al., 2011) on synthetic data (Sections 4.1 and 4.2). We consider different settings to study the robustness of the performances along (i) the number of available observations, (ii) the size of the network, (iii) the distribution of the endogenous noise used to generate data. Our empirical assessment shows that SS-CASTLE compares favorably with all other single-scale baselines, while also sensibly reducing the computational cost.

Notation. We denote by $\mathbb{N}_0$ the set of natural numbers including zero. We indicate with $[X]$, $X \in \mathbb{N}$, the range of the numbers from 1 to X and with $[X]_0$ that from 0 to X. We denote scalars by lowercase letters x, vectors by lowercase bold letters $\mathbf{x}$, and matrices with uppercase bold letters $\mathbf{X}$. Finally, we denote with $\| \cdot \|_F$ the Frobenius norm of a matrix, with $Tr(\cdot)$ its trace, and $\circ$ represents the Hadamard product.

2 Problem formulation

Let us consider a data set $\mathbf{Y} \in \mathbb{R}^{T \times N}$ composed by N time series of length $T = 2^D$, for some $D \in \mathbb{N}$. Let $y_i[t]$ be the value assumed by the i-th time series at time t, and let $\mathcal{P}_{i,l}$ denote the set of parents (in the DAG representation) of $y_i[t]$, with lag $l \in \mathbb{N}_0$. In the single-scale causal structure learning problem for time series, we are interested in understanding whether the considered time series admits a *functional representation* in which $y_i[t]$ depends on a set of parent variables, up to a finite lag L:

$$y_i[t] = f^i \left(\mathcal{P}_{i,L}, \ldots, \mathcal{P}_{i,0}, \epsilon_i[t] \right), \quad i \in [N], \tag{1}$$

where $\epsilon_i[t]$ represents either additive noise, statistically independent of the i-th time series, or a possible model mismatch, occurring at time t. It is worth noticing that the set of parents $\mathcal{P}_{i,l}$ can vary with l. To distinguish causes from effects, the system of Equations (1) must admit a representation based on a DAG.

(a)   (b)

Figure 1: a Example of SSCG with $N = 3$ and maximum lag order $L = 2$; b Example of MSCG with $N = 3$, $D = 3$ time scales and maximum lag order $L = 2$.

As far as lagged interactions are concerned, since we cannot observe causal effects from present to past, $\mathcal{P}_{i,l}$ may contain $y_i[t - l]$, with $l > 0$. In other words, time ordering provides lagged causal connections with implicit causal direction. However, when we look at instantaneous interactions, if we represent each $\mathcal{P}_{i,0}$ over a graph, then the overall graph must be acyclic, otherwise it would be impossible to define the direction of the causal relation.

By limiting our attention to linear dependencies, the causal inference model (1) can be expressed as:

$$\mathbf{y}[t] = \sum_{l=0}^{L} \mathbf{y}[t - l]\mathbf{W}^l + \boldsymbol{\epsilon}[t], \tag{2}$$

which coincides with the so called SVARM. In Equation (2), $\mathbf{y}[t] := (y_1[t], \ldots, y_N[t]) \in \mathbb{R}^{1 \times N}$ is the row vector containing the values assumed by N time series, at time t; whereas $\mathbf{W}^l \in \mathbb{R}^{N \times N}$, with $l \in [L]_0$ and L being the maximum lag, is the matrix representing the causal relation at lag l, so that $w_{ij}^l \neq 0$ if $y_i[t - l] \in \mathcal{P}_{j,l}$. In particular, $\mathbf{W}^0$ represents instantaneous interactions and its structure is such that, if we map the coefficients of $\mathbf{W}^0$ over the edges of a graph of size N, the resulting graph is *acyclic*. Finally, $\boldsymbol{\epsilon}[t] \in \mathbb{R}^{1 \times N}$ represents a random disturbance or model mismatch at time t. Equation (2) is said to be *structural* since it allows us to express variables (effects) as linear functions of other endogenous variables (causes), considering instantaneous as well as lagged relations, also referred to as *intra-* and *inter-layer* connections, respectively. As an example, Figure 1a shows the *single-scale causal graph* (SSCG) associated with Equation (2), in case of $N = 3$ and $L = 2$. In Figure 1a, the subscript represents the node index while the time lag is given within the square brackets. Notably, the graph represents causal interactions from the past to the present, with instantaneous effects at time t avoiding cycles.

2.1 Multiscale Causal Inference Model Based on Stationary Wavelet Transform

The model represented in Equation (2) and sketched in Figure 1a, although very well known and applied, is however limited because it implicitly assumes that the time scale at which important dependencies show up is that associated with the observation task. As discussed in Section 1, causal dependencies might occur at different time scales. Hence, an intriguing and underexplored research problem involves the scenario where the observed variable $y_i[t]$ in Equation (1) can be represented by a *multiscale functional decomposition*. This means that $y_i[t]$ may be decomposed into contributions $y_i^d[t]$, with $d \in [D]$, each having a representation in the form described in Equation (1) and related to a certain frequency band. Mathematically, by defining

$\mathcal{P}_{i,l}^d$ as the parent set of $y_i[t]$ at the d-th time scale, we can express $y_i[t]$ as

$$y_i[t] = \sum_{d=1}^{D} f^{i,d}\left(\mathcal{P}_{i,L}^d, \ldots, \mathcal{P}_{i,0}^d, \epsilon_{i,d}[t]\right), \tag{3}$$

where $\epsilon_{i,d}[t]$ represents an endogenous noise associated with the d-th time scale. Thus, in the case of linear multiscale causal dependencies, it would be beneficial to enhance the SVARM with a multiscale modeling approach.

To develop our multiscale causal inference model, we apply a wavelet decomposition to the observed data set $\mathbf{Y}$. Each row $\mathbf{y}[t]$ of the data set represents a sample collected at the timestamp $t \cdot \Delta t$, where Δt is the time interval between consecutive samples. The wavelet decomposition of level $D-1$ transforms each time series $\mathbf{y}_i$ into $D-1$ vectors of wavelet coefficients and an additional vector of scaling coefficients (see Percival & Mofjeld, 1997 for details). The d-th wavelet coefficients vector corresponds to the variations of $\mathbf{y}_i$ at time scale $2^{d-1} \cdot \Delta t$, representing the frequency band $[1/2^{d+1}, 1/2^d]$. These wavelet coefficients vectors capture the input signal variations over time scales ranging from Δt to $2^{D-2} \cdot \Delta t$, corresponding to frequencies from $1/2^D$ to $1/2$. The scaling coefficients vector contains information about variations over the scale 2^{D-1} and coarser scales, representing frequencies slower than $1/2^D$. Our notation assigns the finest scale ($d = 1$) and the coarsest scale ($d = D$) accordingly.

While the proposed model is flexible and can accommodate various types of wavelet decomposition (Percival & Mofjeld, 1997), our study found that the *stationary wavelet transform* (SWT) (Nason & Silverman, 1995) has the best performance for the learning task. In our notation, $\mathbf{y}^d[t] \in \mathbb{R}^N$ represents the SWT at time t and scale d for the N time series, where $d \in [D]$ and D corresponds to the scaling coefficient. The SWT provides non-decimated detail coefficients $\mathbf{y}^d[t]$ at each scale, offering a *translation invariant* representation. This property is advantageous as it captures relevant information without considering the position of the analysis time window. To preserve both odd and even decimations at each decomposition level and avoid unnecessary redundancies, we use an orthogonal filter family (Daubechies wavelets) within the SWT framework. This choice ensures that the time series $y_i^d[t]$ associated with different time scales are orthogonal. Furthermore, due to the orthogonality property, the energy of the input signal is conserved by the transform and distributed across the scales (Percival & Walden, 2000).

Collecting D different scale details into a single vector $\tilde{\mathbf{y}}[t] := [\mathbf{y}^D[t], \mathbf{y}^{D-1}[t], \ldots, \mathbf{y}^1[t]]$ and stacking these row vectors for $t \in [T]$ on side of each other, we build an augmented data set $\widetilde{\mathbf{Y}} \in \mathbb{R}^{T \times \bar{N}}$ with $\bar{N} = DN$. In this matrix, the row vector at timestamp t contains the t-th detail values of scale d for all N input signals, indexed as $(D-d) \cdot N + 1, \ldots, (D-d+1) \cdot N$. Then, we build the block diagonal matrix $\widetilde{\mathbf{W}}^l :=$ block$[\mathbf{W}_l^D, \mathbf{W}_l^{D-1}, \ldots, \mathbf{W}_l^1]$ of size $\bar{N} \times \bar{N}$. Each d-th block $\mathbf{W}_l^d$ in $\widetilde{\mathbf{W}}^l$ represents the causal interactions $w_{ij}^{d,l}$ occurring at scale d with lag $l \in [L]_0$, where $w_{ij}^{d,l} \neq 0$ if and only if $y_i^d[t-l] \in \mathcal{P}_{j,l}^d$. Here, $\mathcal{P}_{j,l}^d$ represents the parent set for time series $\mathbf{y}_j$ at lag l and scale d, which can vary across both graph layers and pages. Then, the resulting multiscale causal inference models reads as:

$$\widetilde{\mathbf{y}}[t] = \sum_{l=0}^{L} \widetilde{\mathbf{y}}[t-l]\,\widetilde{\mathbf{W}}^l + \widetilde{\boldsymbol{\epsilon}}[t], \tag{4}$$

where $\widetilde{\boldsymbol{\epsilon}}[t] \in \mathbb{R}^{1 \times \bar{N}}$ denotes the additive noise term. In the proposed model, the matrix $\widetilde{\mathbf{W}}^0$ must satisfy the acyclicity requirement to set causes apart from effects.

A pictorial example is given in Figure 1b, which depicts a *multiscale causal graph* (MSCG) for $N = 3$ time series, $D = 3$ time scales, and maximum lag $L = 2$. Each layer in the graph corresponds to a specific time lag, while different pages represent different time scales. In the notation used in Figure 1b, the node superscript denotes the scale index (page of the graph), and the subscript indicates the node index. The time lag is indicated within square brackets. Within each page, we observe both inter-layer and intra-layer directed edges, where the latter, similar to the SSCG case, does not form cycles. However, variables may exhibit different interactions at each time resolution. Therefore, when considering interactions across pages, reverse causal relationships between variables can be observed, as shown by the blue and orange arcs in

Figure 1b. Additionally, due to the use of an orthogonal wavelet family, there are no arcs between pages. Thus, Figure 1b represents a multiscale DAG that incorporates both instantaneous and lagged linear causal relations at different time scales. Each page of the graph is an SSCG at a specific time resolution.

2.2 Optimization Problem Statement

The multiscale causal inference problem aims at learning the matrices $\widetilde{\mathbf{W}}^l$, $l \in [L]_0$, in Equation (4) from data. To ensure the acyclicity of the estimated MSCG, the inferred matrices of causal effects $\widetilde{\mathbf{W}}^l$ must entail a DAG. However, learning DAGs from observational data is a combinatorial problem and, without any restrictive assumption, it has been shown to be NP-hard (Chickering et al., 2004). In our case, since we cannot observe edges coming from the present to the past, lagged causal relationships encompassed in the matrices $\widetilde{\mathbf{W}}^l$ (with $l > 0$) are acyclic by definition. Therefore, the main issue concerns the inference of the matrix $\widetilde{\mathbf{W}}^0$ representing instantaneous causal effects. To handle the acyclicity of $\widetilde{\mathbf{W}}^0$, similarly to DYNOTEARS (Pamfil et al., 2020), we exploit the *dagness* matrix function $h(\mathbf{M}) : \mathbb{R}^{N \times N} \to \mathbb{R}$ proposed by Zheng et al. (2018), who proved that a matrix $\widetilde{\mathbf{W}}^0$ of size $\bar{N} \times \bar{N}$ can be represented as a DAG *if and only if*

$$h(\widetilde{\mathbf{W}}^0) = \mathrm{Tr}\left(e^{\widetilde{\mathbf{W}}^0 \circ \widetilde{\mathbf{W}}^0}\right) - \bar{N} = 0. \tag{5}$$

Using this function as a penalty term, we are now able to formulate the learning task as a continuous, albeit non-convex, optimization problem. To this aim, let us introduce the matrix $\bar{\mathbf{Y}} := [\widehat{\mathbf{Y}}^0, \widehat{\mathbf{Y}}^1, \ldots, \widehat{\mathbf{Y}}^L] \in \mathbb{R}^{T \times V}$ (with $V = \bar{N}(L+1)$) containing the matrices of l-shifted observations $\widetilde{\mathbf{Y}}^l \in \mathbb{R}^{T \times \bar{N}}$. Similarly, we build $\bar{\mathbf{W}} := [\widehat{\mathbf{W}}^{0^T}, \widehat{\mathbf{W}}^{1^T}, \ldots, \widehat{\mathbf{W}}^{L^T}]^T \in \mathbb{R}^{V \times \bar{N}}$. For convenience, let us indicate with $\bar{\mathbb{B}}$ the set of matrices having the same structure as $\bar{\mathbf{W}}$, i.e., made up of stacked block diagonal matrices. Then, the proposed multiscale causal structure learning problem can be mathematically cast as:

$$\begin{aligned} \min_{\bar{\mathbf{W}} \in \bar{\mathbb{B}}} \quad & f(\bar{\mathbf{W}}) + \lambda ||\bar{\mathbf{W}}||_1 \\ \text{subject to} \quad & h(\widetilde{\mathbf{W}}^0) = \mathrm{Tr}\left(e^{\widetilde{\mathbf{W}}^0 \circ \widetilde{\mathbf{W}}^0}\right) - \bar{N} = 0, \end{aligned} \tag{6}$$

where

$$f(\bar{\mathbf{W}}) = \frac{1}{2} \left\| \widetilde{\mathbf{Y}} - \bar{\mathbf{Y}}\bar{\mathbf{W}} \right\|_F^2.$$

The ℓ_1 norm penalty is used in Problem (6) to enforce sparsity of the aggregated causal matrix $\bar{\mathbf{W}}$, with a tunable parameter $\lambda > 0$. Here, differently from already proposed ICA-based estimation procedures (Hyvärinen et al., 2010; Moneta et al., 2013), the matrices of causal coefficients are learnt simultaneously. Despite the convexity of the objective function, Problem (6) is non-convex due to the presence of the acyclicity constraint $h(\widetilde{\mathbf{W}}^0) = 0$. In the next section, we derive an efficient method to solve Problem (6).

3 The MS-CASTLE Algorithm

To find a local solution of Problem (6) or, more precisely, a point that satisfy the Karush-Kuhn-Tucker (KKT) conditions, we exploit the computational efficiency of ADMM (Boyd et al., 2011). To this aim, we recast Problem (6) in the following equivalent manner, introducing the auxiliary matrix $\mathbf{Z} \in \mathbb{R}^{V \times \bar{N}}$, and obtaining

$$\begin{aligned} \min_{\bar{\mathbf{W}} \in \bar{\mathbb{B}}} \quad & f(\bar{\mathbf{W}}) + \lambda ||\mathbf{Z}||_1 \\ \text{subject to} \quad & h(\widetilde{\mathbf{W}}^0) = \mathrm{Tr}\left(e^{\widetilde{\mathbf{W}}^0 \circ \widetilde{\mathbf{W}}^0}\right) - \bar{N} = 0, \\ & \bar{\mathbf{W}} - \mathbf{Z} = \mathbf{0}_{V \times \bar{N}} \ . \end{aligned} \tag{7}$$

Let us now denote by $\bar{\mathbf{w}} = vec(\bar{\mathbf{W}}) \in \mathbb{R}^{V\bar{N}}$, and $\mathbf{z} = vec(\mathbf{Z}) \in \mathbb{R}^{V\bar{N}}$. Then, following the scaled ADMM approach (Boyd et al., 2011), and letting α and β be the Lagrange multipliers associated with the equality constraints of Problem (7), we introduce the following *augmented lagrangian* (AUL) function:

$$\mathcal{L}_\rho\left(\bar{\mathbf{W}}, \mathbf{z}, \alpha, \boldsymbol{\beta}\right) = f(\bar{\mathbf{W}}) + \alpha h\left(\widetilde{\mathbf{W}}^0\right) + \lambda||\mathbf{z}||_1 + \frac{\rho}{2}g(\bar{\mathbf{w}}, \mathbf{z}, \boldsymbol{\beta}), \tag{8}$$

where $g(\bar{\mathbf{w}}, \mathbf{z}, \boldsymbol{\beta}) = \frac{\rho}{2}\|\bar{\mathbf{w}} - \mathbf{z} + \boldsymbol{\beta}\|_2^2 - \frac{\rho}{2}\|\boldsymbol{\beta}\|^2$, and $\rho > 0$ is a tunable positive coefficient. The ADMM algorithm proceeds by iteratively minimizing the AUL function with respect to the primal variables $\bar{\mathbf{W}}$, $\mathbf{z}$, while maximizing it with respect to the dual variables α and $\boldsymbol{\beta}$, looking for saddle points of the AUL. However, while the AUL function is strongly convex w.r.t. $\mathbf{z}$, and naturally concave w.r.t. α and $\boldsymbol{\beta}$, it is non-convex w.r.t. $\bar{\mathbf{W}}$, due to the presence of the non-convex dagness function $h\left(\widetilde{\mathbf{W}}^0\right)$ in Equation (8). To handle this non-convexity issue, following the idea of linearized ADMM methods (Yang & Yuan, 2013; Goldfarb et al., 2013), we substitute the non-convex dagness function $h\left(\widetilde{\mathbf{W}}^0\right)$ in the AUL with its linearization around the current value $\widetilde{\mathbf{W}}_k^0$ assumed at each iteration k, i.e.,

$$\bar{h}\left(\widetilde{\mathbf{W}}^0; \widetilde{\mathbf{W}}_k^0\right) = h\left(\widetilde{\mathbf{W}}_k^0\right) + \mathrm{Tr}\left(G(\widetilde{\mathbf{W}}_k^0)^T(\widetilde{\mathbf{W}}^0 - \widetilde{\mathbf{W}}_k^0)\right), \tag{9}$$

where $G(\widetilde{\mathbf{W}}^0)$ represents the matrix-gradient of function $h\left(\widetilde{\mathbf{W}}^0\right)$. Then, substituting Equation (9) into $h\left(\widetilde{\mathbf{W}}^0\right)$, we obtain the following approximated AUL:

$$\overline{\mathcal{L}}_\rho\left(\bar{\mathbf{W}}, \mathbf{z}, \alpha, \boldsymbol{\beta}; \widetilde{\mathbf{W}}^0\right) = f(\bar{\mathbf{W}}) + \alpha\bar{h}\left(\widetilde{\mathbf{W}}^0; \widetilde{\mathbf{W}}_k^0\right) + \lambda||\mathbf{z}||_1 + \frac{\rho}{2}g(\bar{\mathbf{w}}, \mathbf{z}, \boldsymbol{\beta}), \tag{10}$$

which is now strongly convex w.r.t. $\widetilde{\mathbf{W}}^0$, while preserving the first-order optimality conditions of the AUL in Equation (8) around the current approximation point $\widetilde{\mathbf{W}}_k^0$. As a result, any point satisfying the Karush-Kuhn-Tucker (KKT) conditions using the approximated AUL in Equation (10), satisfies also the KKT conditions of the original Problem (7). Hinging on this fact, we now apply ADMM to the approximated AUL in Equation (10). Then, letting $\widetilde{\mathbf{W}}_k^0$, $\mathbf{z}_k$, α_k, and $\boldsymbol{\beta}_k$ be the current guesses of the primal and dual variables at time k, we obtain the following set of recursions:

$$\bar{\mathbf{W}}_{k+1} = \underset{\bar{\mathbf{W}} \in \bar{\mathbb{B}}}{\arg\min} f(\bar{\mathbf{W}}) + \alpha_k\mathrm{Tr}\left(G(\widetilde{\mathbf{W}}_k^0)^T\widetilde{\mathbf{W}}^0\right) + \frac{\rho}{2}||\bar{\mathbf{w}} - \mathbf{z}_k + \boldsymbol{\beta}_k||_2^2 \tag{11a}$$

$$\mathbf{z}_{k+1} = \underset{\mathbf{z}}{\arg\min} \lambda||\mathbf{z}||_1 + \frac{\rho}{2}||\bar{\mathbf{w}}_{k+1} - \mathbf{z} + \boldsymbol{\beta}_k||_2^2 \tag{11b}$$

$$\alpha_{k+1} = \alpha_k + \gamma\, h\left(\widetilde{\mathbf{W}}_{k+1}^0\right) \tag{11c}$$

$$\boldsymbol{\beta}_{k+1} = \boldsymbol{\beta}_k + \bar{\mathbf{w}}_{k+1} - \mathbf{z}_{k+1} \tag{11d}$$

The first step in Procedure (11) is the minimization of a strongly convex quadratic function, subject to structure constraints $\bar{\mathbf{W}} \in \bar{\mathbb{B}}$, i.e., simple linear constraints on the elements of $\bar{\mathbf{W}}$. We perform this minimization using the L-BFGS-B algorithm (Byrd et al., 1995), i.e., a variation of the Limited-memory Broyden–Fletcher–Goldfarb–Shanno method that handles box constraints. The second step in Procedure (11) can instead be computed in closed form as (Boyd et al., 2011)

$$\mathbf{z}_{k+1} = \mathcal{S}_{(\lambda/\rho)}\left(\bar{\mathbf{w}}_{k+1} + \boldsymbol{\beta}_k\right), \tag{12}$$

where $\mathcal{S}_\delta(x) = \mathrm{sign}(x) \cdot \max(x - \delta, 0)$ is the element-wise soft-thresholding function, used to enforce sparsity of the causal matrix representations. The third step in Procedure (11) performs a gradient ascent step to maximize the function in Equation (10) with respect to α, using a (possibly time-varying) step-size γ. Similar arguments then hold for the fourth step of Procedure (11). All the steps are then summarized in Algorithm 1, which we term as MS-CASTLE.

Remark: Algorithm 1 can be easily customized to solve Equation (2), where we simply ignore the multiresolution analysis. With regards to Algorithm 1, it simply means to skip line 2. This leads to the aforementioned SS-CASTLE algorithm, which applies to a particular sub-case of Problem (6), in which we have: (i) $\widetilde{\mathbf{Y}} = \mathbf{Y}$; (ii) $\bar{\mathbf{Y}} := [\mathbf{Y}^0, \mathbf{Y}^1, \ldots, \mathbf{Y}^L] \in \mathbb{R}^{T \times N(L+1)}$; (iii) $\bar{\mathbf{W}} := [\mathbf{W}^{0^T}, \mathbf{W}^{1^T}, \ldots, \mathbf{W}^{L^T}]^T \in \mathbb{R}^{N(L+1) \times N}$, where $\mathbf{W}^l \in \mathbb{R}^{N \times N}$ are the matrices of causal coefficients of Equation (2).

Algorithm 1 MS-CASTLE

1: **procedure** MS-CASTLE($\mathbf{Y}, L, \lambda, \rho, \gamma, r, t, \gamma^{\max}, \text{maxiter}$)
2:     $\widetilde{\mathbf{Y}} \leftarrow$ Apply SWT to $\mathbf{Y}$
3:     $\bar{\mathbf{Y}} \leftarrow [\widetilde{\mathbf{Y}}^0, \widetilde{\mathbf{Y}}^1, \ldots, \widetilde{\mathbf{Y}}^L]$
4:     Initialize $\bar{\mathbf{W}}, \mathbf{Z}, \alpha, \boldsymbol{\beta}$
5:     **while** k < maxiter & $h_k > t$ **do**
6:         Find $\bar{\mathbf{W}}_{k+1}$ solving Problem (11a)
7:         $h_{k+1} \leftarrow h\left(\bar{\mathbf{W}}_{k+1}\right)$
8:         **if** $h_{k+1}/h_k > r$ **then**
9:             $\gamma \leftarrow 10 \cdot \gamma$ $\triangleright \; \gamma \in (0, \gamma^{\max})$
10:        $\mathbf{z}_{k+1} \leftarrow \mathbf{S}_{(\lambda/\rho)}\left(\bar{\mathbf{w}}_{k+1} + \boldsymbol{\beta}_k\right)$ $\triangleright$ Soft-thresholding
11:        $\alpha_{k+1} \leftarrow \alpha_k + \gamma \cdot h_{k+1}$
12:        $\boldsymbol{\beta}_{k+1} \leftarrow \boldsymbol{\beta}_k + \bar{\mathbf{w}}_{k+1} - \mathbf{z}_{k+1}$
13:     **return** $\bar{\mathbf{W}}$

Initialization. Regarding the initialization of $\bar{\mathbf{W}}$ and $\mathbf{Z}$, they must be initialized in order to satisfy the primal feasibility conditions of Problem (6), i.e, to satisfy the two constraints. A possible choice is to set them equal to zero. Regarding the dual variables of the augmented Lagrangian in Equation (8), α and $\boldsymbol{\beta}$, since they concern equality constraints, they do not need to satisfy any specific condition. Thus, they might be initialized to zero as well.

AUL parameters. The hyper-parameters ρ and γ represent the augmented Lagrangian penalty parameters that can be viewed as the equivalent of dual-ascent step sizes in ADMM procedure. Larger values of these step sizes result in greater penalties for constraints' violations (i.e., primal feasibility). In our case, as in Zheng et al. (2018), the increase in γ is a practical way to manage the violation of the acyclicity constraint. Consequently, it determines the speed of convergence of the proposed algorithm.

Computational cost per iteration. Let us consider w.l.o.g. the single-scale case. In fact, by considering only the active parameters to optimize, the cost of the multiscale case is simply D times that of the single-scale. To solve Equation (11a), we apply L-BFGS-B to an objective function that has a cost of $\mathcal{O}(N^2)$ operations when $T \sim N$ and $L \ll N$. In fact: (i) $f(\bar{\mathbf{W}})$ requires the computation of the product $\bar{\mathbf{Y}}\bar{\mathbf{W}}$ (which costs $\mathcal{O}(N^2)$), plus TN subtractions and the calculation of the squared Frobenius norm (which costs $\mathcal{O}(TN)$); (ii) $\text{Tr}\left(G(\widetilde{\mathbf{W}}_k^0)^T \widetilde{\mathbf{W}}^0\right)$ requires $\mathcal{O}(N^2)$ operations to calculate the product and $\mathcal{O}(N^2)$ operations for the trace; (iii) $||\bar{\mathbf{w}} - \mathbf{z}k + \boldsymbol{\beta}k||_2^2$ requires $\mathcal{O}(N^2)$ additions and subtractions plus $\mathcal{O}(N^2)$ operations for the squared ℓ_2-norm. To solve Equation (11b), we apply the element-wise soft-thresholding operator to a vector of size $N^2(L+1)$. Therefore, the cost is $\mathcal{O}(N^2)$ operations. To solve Equation (11c), we need to compute the dagness function of an $N \times N$ matrix, which has a cost of $\mathcal{O}(N^3)$ (Zheng et al., 2018). Finally, solving Equation (11d) costs $\mathcal{O}(N^2)$ operations.

In the next section, we illustrate the performance of MS-CASTLE and SS-CASTLE, comparing them with alternative methods available in the literature.

4 Numerical Results

In this section, we start showing the advantages of SS-CASTLE (i.e., the customization of the proposed MS-CASTLE method to temporal causal structure analysis) over existing alternative methods in solving Equation (2). More specfically, Section 4.1 shows that, when compared to DYNOTEARS (Pamfil et al., 2020), which aims to solve the same optimization problem, SS-CASTLE benefits from the linearization procedure described above to reduce the computational cost of each iteration while preserving performance. In addition, Section 4.2 illustrates how SS-CASTLE outperforms both VAR-ICALiNGAM and VAR-DirectLiNGAM when we sample $\boldsymbol{\epsilon}[t]$ from a p-generalized normal distribution, with $p \in \{1, 1.5, 2, 2.5, 100\}$. Here, we evaluate the behavior of SS-CASTLE along the size of the network N and the number of samples T as well. Finally,

Figure 2: Number of iterations (left) and computational time (right) to solve Equation (2) shown by DYNOTEARS (purple) and SS-CASTLE (pink).

in Section 4.3 we assess the performance of MS-CASTLE on multiscale synthetic data. Also in this case, we test the performance of our method along N, T, and in both Gaussian and non-Gaussian settings. In addition, we study how different choices of wavelets affect the performance of MS-CASTLE.

4.1 Comparison with DYNOTEARS

Here we provide a comparison between SS-CASTLE and DYNOTEARS (Pamfil et al., 2020). We test the two methods over synthetic data, so that the ground truth is known. Our goal is to compare empirically the computational time needed to the two alternative methods to estimate the causal matrices in Equation (2) with a similar accuracy. Actually, from a theoretical point of view, considering the analysis of computational cost per iteration of our method reported in Section 3, we have that SS-CASTLE reduces the computational cost of DYNOTEARS in two ways. Firstly, the linearization of the dagness function lowers the computational cost required to update $\bar{\mathbf{W}}$. In fact, in our case, the calculation of the objective function requires $\mathcal{O}(N^2)$ operations, compared to the $\mathcal{O}(N^3)$ required by DYNOTEARS. Secondly, to impose regularization on the ℓ_1 norm of causal coefficients, SS-CASTLE leverages the element-wise soft-thresholding operator. In contrast, similar to Zheng et al. (2018), DYNOTEARS uses the splitting trick, writing $\bar{\mathbf{W}} = \bar{\mathbf{W}}_+ - \bar{\mathbf{W}}_-$, where $\bar{\mathbf{W}}_+ \geq 0$ and $\bar{\mathbf{W}}_- \geq 0$ (having the same dimensions as $\bar{\mathbf{W}}$), thus doubling the number of parameters to be estimated.

4.1.1 Data Generation

We generate synthetic data according to Equation (2). Specifically, we set $L = 1$ and we assume that each $\epsilon_i[t] \sim N\left(0, \sigma_i^2\right)$ with $\sigma_i^2 \in [1, 2]$. Moreover, we set the number of samples $T = 1000$ and we pick $N \in \{10, 30, 50, 100\}$. For each of the four possible values of the number of nodes, we simulated 100 data sets. Regarding the causal matrices, we generate them by adopting the same procedure illustrated by Hyvärinen et al. (2010). To manage the level of the sparsity of $\mathbf{W}^0$ and $\mathbf{W}^1$, we introduce the parameter $s \in (0, 1)$. The latter is used as a parameter of a Bernoulli distribution, more precisely $\mathcal{B}(1 - s)$, which controls the number of nonzero coefficients of the causal matrices. As the number of nodes N grows, we increase the sparsity of the causal structure. More specifically, the combinations (N, s) used in the experiments below are $\{(10, .80), (30, .85), (50, .90), (100, .95)\}$.

4.1.2 Results

Figure 2 displays the number of iterations (left) and computational time (right) needed to solve Equation (2), as a function of the number of nodes, by DYNOTEARS (purple) and SS-CASTLE (pink), respectively. On the left of Figure 2, we report a swarm plot in which, given a certain number of nodes, each point represents the number of iterations required by each algorithm to retrieve the solution. In accordance with the data generating process described above, for each value of N we have 100 points per algorithm. Therefore, given a certain value of N and a specific number of iterations n, the number of points reported in horizontal represents the number of data set (composed by N time series) in which the algorithm required n iterations to solve the problem.

On the right of Figure 2, we provide a violin plot that depicts, for each value of N, the histogram of the computational time (measured in seconds) needed by each algorithm to solve the problem. Moreover, dashed lines within the histogram represent quartiles. From Figure 2 (left), we see that, even though SS-CASTLE needs more iterations to converge, SS-CASTLE significantly reduces the overall computational time to converge. Furthermore, we also observe that the larger the network size, the greater the gain. Hence, in accordance with the theoretical insights highlighted above, we conclude that SS-CASTLE decreases the computational cost associated with each iteration while preserving performance (see Appendix A).

4.2 Comparison with Linear Non-Gaussian Methods

We compared the performance of SS-CASTLE and of two major linear non-Gaussian methods, i.e., VAR-ICALiNGAM and VAR-DirectLiNGAM, on synthetic data sets as well. More in detail, the latter two models rely upon the assumption of non-Gaussianity of $\epsilon[t]$ in Equation (2). VAR-ICALiNGAM belongs to the family of ICA-based methods: first it fits a VAR model to recover lagged causal interactions and then it employs FastICA (Hyvarinen, 1999) on VAR residuals to uncover instantaneous relationships. In the past, several ICA-based algorithms have been developed. However, as shown in Moneta et al. (2020), previous models are equivalent in terms of performance. Regarding VAR-DirectLiNGAM, it was proposed in order to solve the possible convergence issues of ICA-based methods (Himberg et al., 2004) and it is guaranteed to retrieve the right solution of the problem if the model assumptions are satisfied and the sample size is very large. In the experiments below, in order to fit the aforementioned models, we use the `lingam` Python package[1] made available from the authors.

4.2.1 Data Generation

We generated synthetic data by using Equation (2), in which we set $L = 1$. Moreover, we conducted an extensive simulation study in order to assess the robustness of all the methods in different settings. In particular, we varied the features of the generated data sets as follows. Firstly, we use different data set sizes, $T \in \{100, 500, 1000\}$. By varying the number of samples, we can inspect the sensitivity with respect to the data set size of the tested algorithms. The latter aspect is relevant in several fields, especially when the system at a hand shows non-stationarity. For instance, this is the case in finance, where practitioners usually deal with a small number of historical observations due to the continuous evolution of financial markets. Secondly, we vary the network size, $N \in \{10, 30, 50\}$. Concerning the level of sparsity and the generation of the causal matrices, we adopt the same methodology described in Section 4.1.1. Last but not least, we sample $\epsilon[t]$ from a p-generalized normal distribution, with $p \in \{1, 1.5, 2, 2.5, 100\}$. The p-generalized normal distribution is defined as follows (Kalke & Richter, 2013).

Definition 4.1 (p-generalized normal distribution). Let us consider $x \in \mathbb{R}$, $p \in \mathbb{R}^+$. Therefore, the p-generalized normal distribution has density function equal to

$$f_p(x) = \frac{p^{1-1/p}}{2\Gamma(1/p)} \exp\left[-\frac{|x|^p}{p}\right],\tag{13}$$

where Γ is the gamma function.

The parameter p determines the rate of decay of Equation (13). More in detail: (i) $p = 1$ corresponds to a Laplace distribution; (ii) $p = 1.5$ is the super-Gaussian case; (iii) for $p = 2$ we get the normal distribution; (iv) $p = 2.5$ is the sub-Gaussian case; (v) for $p = 100$ we obtain approximately a uniform distribution. Therefore, as p diverges from 2, the non-normality of $\epsilon[t]$ is enhanced. For each combination of the parameters, we generate 100 data sets.

4.2.2 Results

Before testing SS-CASTLE on the generated data, we fine-tune the sparsity strength λ onto separate data sets generated according to the procedure explained above. More precisely, we let λ assume values in the set $\{.001, .005, .01, .05, .1, .5\}$ and, for each combination $(T, N, p)_i$, we chose the best value according to F1-score

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[1]The package is available at `https://github.com/cdt15/lingam`.

Figure 3: Comparison with VAR-DirectLiNGAM and with VAR-ICALiNGAM in the estimation of the causal matrices $\mathbf{W}^0$ (top) and $\mathbf{W}^1$ (bottom). Each subfigure depicts box plots for the F1-score when a $(N, T) \in \{30\} \times \{100, 500, 1000\}$ and b $(N, T) \in \{10, 30, 50\} \times \{1000\}$.

and SHD (structural Hamming distance). Due to the needed computational time, for the case $N = 50$ we restrict the possible values of λ to $\{.01, .05, .1, .5\}$. The latter restriction does not impact the analysis since our objective is not to find the optimal value of the hyper-parameter, but rather to set the latter in a data-driven manner. The chosen values for λ are given in Appendix B.

Sensitivity to data set size. Figure 3a depicts the performance comparison in the learning of $\mathbf{W}^0$ (top) and $\mathbf{W}^1$ (bottom). For readability, we provide only the results in case of $N = 30$ nodes. Results are qualitatively equivalent in the other two cases. As we can see from Figure 3a, SS-CASTLE outperforms VAR-DirecLiNGAM and VAR-ICALiNGAM in term of F1-score. In addition, Appendix C provides results for SHD metric. Concerning the learning of $\mathbf{W}^0$, even though VAR-DirectLiNGAM shows a slightly better performance than VAR-ICALiNGAM in case of strongly non-Gaussian settings ($p = 1$ and $p = 100$) and larger data sets ($T = 500$ and $T = 1000$), it tends to suffer more when the non-Gaussianity assumption becomes violated and a lower number of samples is available. The latter behaviour is consistent with DirectLiNGAM model assumptions. In accordance with the problem formulation (see Section 3), SS-CASTLE does not show any dependence on p, and requires a smaller number of data to converge towards a more accurate solution.

Regarding the matrix of lagged causal effects $\mathbf{W}^1$, differently from the considered non-Gaussian methods, SS-CASTLE contemporaneously estimates inter and intra-layer connections. In addition, we see that all models tend to be more accurate in retrieving the lagged interactions. Please notice that, given the time ordering, $\mathbf{W}^1$ is acyclic by definition. Therefore, all entries could be different from zero. This means that in case of $N = 30$ and $s = 0.85$, on average we have 135 nonzero coefficients.

Sensitivity to network size. Figure 3b shows the comparison of models performance in the estimation of the causal relationships along N. For readability, we provide only the results for the case $T = 1000$. The results are qualitatively equivalent in the remaining two cases. In addition, Appendix C provides results for SHD metric. Looking at the case of instantaneous interactions (top row), at a first glance we notice the higher error variance in the box plots related to F1-score, when $N = 10$, across all models. However, even though F1-score is a normalized metric, this is an effect of the small number of instantaneous causal connections. Indeed, in case of $N = 10$ and $s = .80$, on average the ground truth $\mathbf{W}^0$ has only 9 entries different from zero. As a consequence, a single mistake weights more. Overall, from Figure 3b, we can see how SS-CASTLE outperforms the other methods. Moreover, we do not appreciate a decrease in performance when the number of nodes increases. In addition, SS-CASTLE proves to be robust to changes in the value of p.

Regarding lagged causal connections (bottom row), the models tend to perform better than in the case of instantaneous relations. We underline that, in case of $N = 10$, we do not observe the same error variance as

above. Indeed, with the same level of sparsity s, on average $\mathbf{W}^1$ has approximately twice as many non-zero entries than $\mathbf{W}^0$. Overall, we notice that non-Gaussian algorithms tend to suffer when the number of nodes increases. Our results show that VAR-ICALiNGAM tends to be more robust than VAR-DirectLiNGAM as the non-Gaussianity assumption turns out to be violated. Also in this case, SS-CASTLE does not show any decrease in performance while varying p. In addition, it achieves high performance in case of larger networks as well.

4.3 Performance of MS-CASTLE on Synthetic Data

Here we provide the empirical assessment of MS-CASTLE. Analogously to the previous section, we evaluate the performance of our method when varying the network size, the data set size, and the distribution of the random disturbances. In addition, we are interested in understanding how the choice of a wavelet in the decomposition phase affects the performance of MS-CASTLE. Therefore, we compare different versions of MS-CASTLE. First, we consider the case in which MS-CASTLE receives as input the perfect decomposition of the time series, i.e., $\tilde{\mathbf{y}}[t]$ used in the data generation process. This case represents an upper bound for our method, as there are no errors induced by the wavelet transform. We refer to this version as *MS-CASTLE opt. dec.*. Next, we consider the case in which MS-CASTLE uses the same wavelet used in the generative process, namely Daubechies with a filter of length 10 (*MS-CASTLE swt db5*). We then test two other versions in which we use a different wavelet than the one used in the generative process, namely Daubechies with filters of length 6 (*MS-CASTLE swt db3*) and 14 (*MS-CASTLE swt db7*).

4.3.1 Data Generation

We generate multiscale observable data $\mathbf{Y} \in \mathbb{R}^{T \times N}$ determined by an underlying multiscale causal structure according to the proposed model in Equation (3) and Equation (4). First, we sample an i.i.d. noise $\boldsymbol{\epsilon}[t] \in \mathbb{R}^N$ from a p-generalized normal distribution. Next, w.l.o.g. we decompose $\boldsymbol{\epsilon}[t]$ with a DWT using as wavelet Daubechies with filter length 10 and considering $D = 4$, thus obtaining $\widetilde{\boldsymbol{\epsilon}}[t]$ in Equation (4). Hence, we generate $\tilde{\mathbf{y}}[t]$ by imposing a multiscale causal structure containing both lagged ($L = 1$) and instantaneous interactions on four different frequency bands (see Appendix D). Finally, we obtain $\mathbf{y}[t]$ by summing the contributions from the time scales, in accordance with Equation (3) and in general with the synthesis capability associated with the wavelet transform (Percival & Mofjeld, 1997).

In the experiments, we perform the following analysis: (i) we study the sensitivity to the size of the graph we vary $N \in \{5, 10, 30\}$; (ii) we assess possible dependencies on the number of samples we vary $T \in \{128, 512, 8192\}$; finally (iii) we deal with the Gaussian $p = 2$ and non-Gaussian $p = 1$ cases. For each of these settings, we simulate 20 data sets.

4.3.2 Results

Figure 4 depicts the F1-score obtained by the considered versions of MS-CASTLE on the settings described above. The values of λ used in the experiments are given in Appendix B, while Appendix E provides other results concerning the SHD. Overall, MS-CASTLE achieves the best performance when it receives as input $\tilde{\mathbf{y}}[t]$ used in the generative process (perfect decomposition of the observed time series). Furthermore, for the same network size N, the F1 score improves as the number of samples T increases. In contrast, we do not notice any dependence of MS-CASTLE on either the number of time series N or the noise distribution (Gaussian vs. non-Gaussian setting). In addition, the results show that the performance of MS-CASTLE is robust to the choice of wavelet used to decompose the input time series.

5 Causal Structure Analysis of Financial Markets

In this section, we apply the proposed technique to infer the causal structure of financial markets. We consider data concerning 15 global equity markets at daily frequency. To focus on covid-19 pandemic period, we restrict our attention to observations from January 2020, the 2nd to April 2021, the 30th. In our analysis, we deal with the following markets: *All Ordinaries Index* (AOR, Australia), *Hang Seng Index* (HSI, Hong Kong), *Nikkei 225 Index* (NKX, Japan), *Shanghai Composite Index* (SHC, Shanghai), *Straits Times Index*

Figure 4: Comparison of different versions of MS-CASTLE in terms of F1-score, obtained in the experimental settings described above. Subplots on the top refer to the Gaussian setting, whereas those on the bottom to the non-Gaussian one. Subplots on the left refer to the case $N = 5$, those on the center to $N = 10$, and those on the right to $N = 30$. Dashed lines represent the inter-quartile range.

(STI, Singapore), *TAIEX Index* (TWSE, Taiwan), *DAX Index* (DAX, Germany), *FTSE MIB Index* (FMIB, Italy), *IBEX Index* (IBEX, Spain), *CAC 40 Index* (CAC, France), *FTSE 100 Index* (UKX, UK), *RTS Index* (RTS, Russia), *Bovespa Index* (BVP, Brazil), *Nasdaq Composite Index* (NDQ, US), *S&P/TSX Composite Index* (TSX, Canada). In particular, we analyze the series of markets risk, as measured by conditional volatility. Hence, the time series of conditional volatility represent our input data set **Y**. Information concerning data source and pre-processing is given in Appendix F.

5.1 Methodological Approach

In this section, we deepen the methodology used to retrieve the causal structure underlying the data, coming from the estimation of the causal matrices in both Equations (2) and (4), and constituted by highly persistent edges. In particular, due to non-convexity of Problem (6), both SS-CASTLE and MS-CASTLE generally converge to stationary points that, possibly, can be different from each other for diverse values of the sparsity-inducing parameter λ. Thus, to reduce this ambiguity, in our analysis we look for solutions of SSCG and MSCG that are as persistent as possible with respect to different values of λ. To this aim, we first choose

(a) SS-CASTLE   (b) MS-CASTLE

Figure 5: Behaviour of regularization to fitting loss ratio along λ for SS-CASTLE (left) and MS-CASTLE (right), where the x axis is given in log scale.

a suitable range for the previous hyper-parameter, looking at the regularization to fitting loss ratio, i.e., the quotient of the division between the second and the first term of the objective function of Problem (6). Figure 5 shows the behavior of the regularization to fitting loss ratio with respect to λ, considering both SS-CASTLE (left) and MS-CASTLE (right). As a meaningful range, we select the values that return a ratio from 0.1 to 1. In this way, we track the change in causal connections when the sparsity-inducing regularization term becomes as important as the model fitting term. Then, from Figure 5, we select (i) $\lambda \in [0.004, 0.04]$ for SS-CASTLE; and (ii) $\lambda \in [0.003, 0.03]$ for MS-CASTLE. For each interval, we pick 10 values for λ.

Once the range of λ is identified, we define the persistence of a causal relation at a threshold $\bar{c}$ as follows. Let us indicate with $\mathbf{r}$ the vector constituted by the regularization to fitting ratios r_k corresponding to the chosen k values of λ. In addition, consider w_{ij}^k as the causal coefficient from node i to j estimated for $\lambda = \lambda_k$. Then, the persistence of the causal coefficient is

$$p_{ij} = \frac{\sum_k \mathbf{1}_{|w_{ij}^k| > \bar{c}} \cdot r_k}{\sum_k r_k}, \tag{14}$$

where $\mathbf{1}_{|w_{ij}^k| > \bar{c}}$ is equal to 1 iff $|w_{ij}^k| > \bar{c}$, and zero otherwise. Equation (14) assigns a higher persistence value to arcs that are present in causal structures estimated from Problem (6) for multiple values of λ. Also, from Equation (14), it holds $p_{ij} \in [0, 1]$. However, the formula does not provide any guarantee regarding the stability of the sign of the causal relation. Indeed, it only considers the presence of an arc and not the value (and therefore the sign) of the causal coefficient associated with the arc. Thus, we define as highly persistent only those edges, with $p_{ij} > 0.95$, which show a stable sign of the corresponding causal coefficient for all values of λ. These edges constitute the causal structures illustrated in the sequel.

5.2   Single-scale Causal Analysis

(a)   (b)

Figure 6: Highly persistent causal matrices for the a single-scale and b multiscale case where $\bar{c} = 0.05$. Red entries represent positive coefficients, whereas blue ones are negative.

To compare single and multiscale approaches, we estimate the causal matrices in both Equations (2) and (4) by using SS-CASTLE and MS-CASTLE, respectively. Here, we focus on learning causal graphs from time series using the aforementioned SS-CASTLE method. Figure 6a shows the signed causal matrix made up of persistent coefficients, where for readability reasons we only report the case of $\bar{c} = 0.05$. Additional results are provided in Appendix G.

In particular, in the matrix shown in Figure 6a the rows represent the parents (sorted according to the timestamp), whereas the columns refer to the caused nodes. In this case, based on BIC criterion, we set $L = 1$. The upper block of the matrix in Figure 6a concerns lagged causal interactions, while the lower one is related

to instantaneous causal effects. In our study we observe that arcs associated with negative causal relations get a weight lower than 0.1 (in module); whereas, most of surviving edges correspond to autoregressive causal effects (see also Appendix G). In addition, we find denser causal connections among European and Asia-Pacific countries. Overall, from the single-scale analysis, we cannot find nodes representing major risk drivers within the network, i.e., the considered equity markets show a similar number of outgoing arcs (i.e., out-degree).

5.3 Multiscale Causal Analysis

We now focus on multiscale causal analysis, where we analyze the first four temporal resolutions, in accordance with the length of our data set, i.e., $T = 336$ observations (see Section 3). In addition, similarly to (Ren et al., 2021), we use Daubechies least asymmetric wavelets with filter length equal to 8. Figure 6b illustrates the highly persistent multiscale causal matrices obtained using the proposed MS-CASTLE method, for the same value of $\bar{c}$ analyzed above. Additional results are provided in Appendix G. For the sake of readability, we show separately the diagonal blocks of $\bar{\mathbf{W}}$ corresponding to different scales, i.e., the only elements of $\bar{\mathbf{W}}$ that can be different from zero in Equation (4) (since no interaction among scales actually takes place). From Figure 6b, we first notice that causal representations at different scales show a diverse level of sparsity and, furthermore, persistent causal relations assume only positive values. More in details, causal interactions are denser at mid-term scales (i.e., 3 and 4, which correspond to 8-16 and 16-32 days, respectively). On the contrary, causal effects turn out to be not persistent at scale 1, which represents a time resolution of 2-4 days. In summary, we found that: (i) the strongest persistent connections appear at scale 3 and 4; (ii) the majority is lagged; and (iii) the most instantaneous relations are associated to weights lower than 0.05 (in module) (see also Appendix G). In addition, we noticed the following behaviors: i) apart from Australia, Asia-Pacific countries are isolated for $\bar{c} > 0.05$; ii) the markets that drive the risk within the network are Brazil, Canada and Italy. The latter finding can be understood by looking at the number of nonzero entries per market across columns, representing the out-degree of each node. More in detail, the impacts of Brazil and Canada spread across all geographical areas, while Italy mainly drives the risk within the Eurozone. Finally, from Figure 6b, we can notice how US displays persistent lagged connections.

5.4 Comparison Between Temporal and Multiscale Analysis

The results presented in Sections 5.2 and 5.3 illustrate that, in case of complex systems such as financial markets, temporal and multiscale analysis might lead to very different conclusions. First of all, the inferred SSCG indicates a persistent causal structure at daily frequency, where the strongest connections are autoregressive lagged causal relations. On the contrary, empowered by information concerning the variation of the original signal at different scales, the MSCG shows that causal structures persist at mid-term scales (i.e., 3 and 4), while at short-term scale causal connections are absent. Thus, we can conclude that, in our case, the mere application of a multiscale-agnostic model leads to a noisy estimate of the causal structure, in which many of the relationships do not persist when decomposing the signal into different temporal resolutions. Also, in MSCG we do not observe negative causal coefficients as in case of SSCG, which are somehow difficult to justify during the considered period, since they indicate that an increase (decrease) in the volatility of a certain equity market causes a decrease (increase) in that of another market.

Finally, and most importantly, multiscale causal analysis allows us to identify the major risk drivers within the network of equity markets during covid-19 pandemic, i.e., Brazil, Canada and Italy. Interestingly, the US stock market, shows only an impact on Australia, together with an autoregressive effect. In particular, the importance of Canada within the network of stock markets has been underlined by (Ren et al., 2021) as well, who conducted a study in terms of partial correlation networks. However, since we deal with causation, our result has stronger implications with respect to the aforementioned work. With regards to Brazil, we see that the corresponding stock index shows the highest volatility (see Appendix F), and that its strongest connections (greater than 0.1) are within the American area (see Appendix G). Last, but not least, Italy has a high impact within the European area.

6 Conclusions and Future Research Directions

In this paper we have proposed a novel method to estimate the structure of linear causal relationships at different time scales. By relying upon wavelet transform and non-convex optimization, MS-CASTLE takes explicitly into consideration behaviors of the system at hand spanning at diverse time resolutions. Differently from existing causal inference methods, MS-CASTLE looks for linear causal relationships among variations of input signals within multiple frequency bands, and across different time lags. We illustrate that the multiscale-agnostic version of MS-CASTLE, named SS-CASTLE, improves in terms of computational efficiency, performance and robustness over the state of the art. In addition, experiments on synthetic data show that the performance of MS-CASTLE increases with samples availability and is robust to the network size, the noise distribution, and the choice of the wavelets.

The study of the risk of 15 global equity markets, during covid-19 pandemic, shows that MS-CASTLE is able to provide useful information about the scales at which causal interactions occur (mid-term scales) and to identify major risk drivers within the system (Brazil, Canada and Italy). We highlight that the obtained results must be framed in the period of the coronavirus outbreak. Our choice was conscious: given the nonstationary nature of financial markets (Schmitt et al., 2013), we focused on a narrow period dominated by the pandemic emergency. Thus, the use of different time windows may lead to the estimation of a different multiscale causal structure. This observation highlights the need to work on the development of causal inference algorithms capable of handling both the multiscale nature of the analyzed system and the nonstationarity of the underlying causal structure (D'Acunto et al., 2021). In this context, the application of Gaussian processes to model the time dependence of the causal structure has led to some advances (Huang et al., 2015).

In addition, the proposed model considers only linear causal relationships: generalisation to nonlinear interactions represents further future work. Here, kernel methods (Shen et al., 2016) and more recently non-linear ICA (Monti et al., 2020) has been used to tackle the estimation task. However, previous works only refer to the single-scale case. Also, in this work we did not consider possible inter-scale cause-effect mechanisms. However, we do not exclude that behaviors of signals at higher frequencies may impact those at lower frequencies and vice versa. So, investigating the existence of such causal relationships represents an interesting future research direction.

Furthermore, we did not establish any identifiability result of the multiscale causal structure. The results that have been established for instantaneous causal relations at a single time scale (Shimizu et al., 2006; Peters et al., 2014; Park & Kim, 2020) do not generalise to the multiscale case due to the possible presence of serial correlation in the noise decomposition. Furthermore, the unobservability of the underlying contribution coming from different time scales is another intriguing element that sets the multiscale case apart from the single-scale case. Hence, we plan to investigate the identifiability of multiscale causal graphs in future work.

Additionally, it would be useful to improve our method for managing multiscale, non-stationary, and possibly nonlinear causal dynamics. Indeed, it is common in different application domains, such as finance, neuroscience, and climatology, to deal with data featured by the previous characteristics.

Finally, the results of the case study show how MS-CASTLE can be used to support portfolio risk management. Indeed, depending on their investment horizon, investors could use the proposed methodology to make risk-aware decisions regarding their portfolios, from a causal perspective and without any prior assumption about the scale of analysis.

References

Mark Alber, Adrian Buganza Tepole, William R Cannon, Suvranu De, Salvador Dura-Bernal, Krishna Garikipati, George Karniadakis, William W Lytton, Paris Perdikaris, Linda Petzold, et al. Integrating machine learning and multiscale modeling—perspectives, challenges, and opportunities in the biological, biomedical, and behavioral sciences. *NPJ digital medicine*, 2(1):1–11, 2019.

Michel Besserve, Bernhard Schölkopf, Nikos K Logothetis, and Stefano Panzeri. Causal relationships between frequency bands of extracellular signals in visual cortex revealed by an information theoretic analysis.

Journal of computational neuroscience, 29:547–566, 2010.

Monica Billio, Mila Getmansky, Andrew W Lo, and Loriana Pelizzon. Econometric measures of connectedness and systemic risk in the finance and insurance sectors. *Journal of Financial Economics*, 104(3):535–559, 2012.

Tim Bollerslev. Generalized autoregressive conditional heteroskedasticity. *Journal of Econometrics*, 31(3): 307–327, 1986.

Stephen Boyd, Neal Parikh, and Eric Chu. *Distributed Optimization and Statistical Learning via the Alternating Direction Method of Multipliers*. Now Publishers Inc, 2011.

Peter Bühlmann, Jonas Peters, Jan Ernest, et al. Cam: Causal additive models, high-dimensional order search and penalized regression. *Annals of Statistics*, 42(6):2526–2556, 2014.

Richard H Byrd, Peihuang Lu, Jorge Nocedal, and Ciyou Zhu. A limited memory algorithm for bound constrained optimization. *SIAM Journal on scientific computing*, 16(5):1190–1208, 1995.

Laurent Calvet and Adlai Fisher. Forecasting multifractal volatility. *Journal of econometrics*, 105(1):27–58, 2001.

David Maxwell Chickering. Optimal structure identification with greedy search. *Journal of Machine Learning Research*, 3(Nov):507–554, 2002.

Max Chickering, David Heckerman, and Chris Meek. Large-sample learning of Bayesian networks is NP-hard. *Journal of Machine Learning Research*, 5, 2004.

Philippe Ciuciu, Patrice Abry, and Biyu J He. Interplay between functional connectivity and scale-free dynamics in intrinsic fMRI networks. *Neuroimage*, 95:248–263, 2014.

Gabriele D'Acunto, Paolo Bajardi, Francesco Bonchi, and Gianmarco De Francisci Morales. The evolving causal structure of equity risk factors. In *Proceedings of the Second ACM International Conference on AI in Finance*, pp. 1–8, 2021.

Gabriele D'Acunto, Gianmarco De Francisci Morales, Paolo Bajardi, and Francesco Bonchi. Multiscale non-stationary causal structure learning from time series data. *arXiv preprint arXiv:2208.14989*, 2022.

Clark Glymour, Kun Zhang, and Peter Spirtes. Review of causal discovery methods based on graphical models. *Frontiers in genetics*, 10:524, 2019.

Donald Goldfarb, Shiqian Ma, and Katya Scheinberg. Fast alternating linearization methods for minimizing the sum of two convex functions. *Mathematical Programming*, 141(1):349–382, 2013.

Mingming Gong, Kun Zhang, Bernhard Schoelkopf, Dacheng Tao, and Philipp Geiger. Discovering temporal causal relations from subsampled data. In *International Conference on Machine Learning*, pp. 1898–1906. PMLR, 2015.

Kazuharu Harada and Hironori Fujisawa. Sparse estimation of linear non-Gaussian acyclic model for causal discovery. *Neurocomputing*, 459:223–233, 2021.

David Heckerman, Dan Geiger, and David M Chickering. Learning Bayesian networks: The combination of knowledge and statistical data. *Machine learning*, 20(3):197–243, 1995.

Johan Himberg, Aapo Hyvärinen, and Fabrizio Esposito. Validating the independent components of neuroimaging time series via clustering and visualization. *Neuroimage*, 22(3):1214–1222, 2004.

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*, 21:689–696, 2008.

Biwei Huang, Kun Zhang, and Bernhard Schölkopf. Identification of time-dependent causal model: A Gaussian process treatment. In *Twenty-Fourth International Joint Conference on Artificial Intelligence*, 2015.

Biwei Huang, Kun Zhang, Yizhu Lin, Bernhard Schölkopf, and Clark Glymour. Generalized score functions for causal discovery. In *Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pp. 1551–1560, 2018.

Biwei Huang, Kun Zhang, Jiji Zhang, Joseph Ramsey, Ruben Sanchez-Romero, Clark Glymour, and Bernhard Schölkopf. Causal discovery from heterogeneous/nonstationary data. *Journal of Machine Learning Research*, 21(89):1–53, 2020.

Aapo Hyvarinen. Fast and robust fixed-point algorithms for independent component analysis. *IEEE Transactions on Neural Networks*, 10(3):626–634, 1999.

Aapo Hyvärinen, Kun Zhang, Shohei Shimizu, and Patrik O Hoyer. Estimation of a structural vector autoregression model using non-Gaussianity. *Journal of Machine Learning Research*, 11(5), 2010.

Jaime Ide, Fábio Cappabianco, Fabio Faria, and Chiang-shan R Li. Detrended partial cross correlation for brain connectivity analysis. *Advances in Neural Information Processing Systems*, 30, 2017.

Joshua Jacobs, Michael J Kahana, Arne D Ekstrom, and Itzhak Fried. Brain oscillations control timing of single-neuron activity in humans. *Journal of Neuroscience*, 27(14):3839–3844, 2007.

Steve Kalke and W-D Richter. Simulation of the p-generalized Gaussian distribution. *Journal of Statistical Computation and Simulation*, 83(4):641–667, 2013.

Rabeh Khalfaoui, Mohamed Boutahar, and Heni Boubaker. Analyzing volatility spillovers and hedging between oil and stock markets: Evidence from wavelet analysis. *Energy Economics*, 49:540–549, 2015.

Lutz Kilian and Helmut Lütkepohl. *Structural vector autoregressive analysis*. Cambridge University Press, 2017.

Jarosław Kwapień and Stanisław Drożdż. Physical approach to complex systems. *Physics Reports*, 515(3-4):115–226, 2012.

Sébastien Lachapelle, Philippe Brouillard, Tristan Deleu, and Simon Lacoste-Julien. Gradient-based neural DAG learning. In *International Conference on Learning Representations*, 2020. URL https://openreview.net/forum?id=rklbKA4YDS.

Lixia Loh. Co-movement of Asia-Pacific with European and US stock market returns: A cross-time-frequency analysis. *Research in International Business and Finance*, 29:1–13, 2013.

Rosario N Mantegna and H Eugene Stanley. *Introduction to econophysics: correlations and complexity in finance*. Cambridge university press, 1999.

Alessio Moneta, Doris Entner, Patrik O Hoyer, and Alex Coad. Causal inference by independent component analysis: Theory and applications. *Oxford Bulletin of Economics and Statistics*, 75(5):705–730, 2013.

Alessio Moneta, Gianluca Pallante, et al. Identification of structural VAR models via independent component analysis: A performance evaluation study. Technical report, Laboratory of Economics and Management (LEM), Sant'Anna School of Advanced Studies, 2020.

Ricardo Pio Monti, Kun Zhang, and Aapo Hyvärinen. Causal discovery with general non-linear relationships using non-linear ICA. In *Uncertainty in Artificial Intelligence*, pp. 186–195. PMLR, 2020.

Guy P Nason and Bernard W Silverman. The stationary wavelet transform and some statistical applications. In *Wavelets and statistics*, pp. 281–299. Springer, 1995.

Ignavier Ng and Kun Zhang. Towards federated Bayesian network structure learning with continuous optimization. In *International Conference on Artificial Intelligence and Statistics*, pp. 8095–8111. PMLR, 2022.

Ignavier Ng, AmirEmad Ghassami, and Kun Zhang. On the role of sparsity and DAG constraints for learning linear DAGs. *Advances in Neural Information Processing Systems*, 33:17943–17954, 2020.

Roxana Pamfil, Nisara Sriwattanaworachai, Shaan Desai, Philip Pilgerstorfer, Konstantinos Georgatzis, Paul Beaumont, and Bryon Aragam. DYNOTEARS: Structure learning from time-series data. In *International Conference on Artificial Intelligence and Statistics*, pp. 1595–1605. PMLR, 2020.

Gunwoong Park and Youngwhan Kim. Identifiability of Gaussian linear structural equation models with homogeneous and heterogeneous error variances. *Journal of the Korean Statistical Society*, 49:276–292, 2020.

Judea Pearl. *Causality*. Cambridge university press, 2009.

Grace CY Peng, Mark Alber, Adrian Buganza Tepole, William R Cannon, Suvranu De, Savador Dura-Bernal, Krishna Garikipati, George Karniadakis, William W Lytton, Paris Perdikaris, et al. Multiscale modeling meets machine learning: What can we learn? *Archives of Computational Methods in Engineering*, 28(3): 1017–1037, 2021.

Donald B Percival and Harold O Mofjeld. Analysis of subtidal coastal sea level fluctuations using wavelets. *Journal of the American Statistical Association*, 92(439):868–880, 1997.

Donald B Percival and Andrew T Walden. *Wavelet Methods for Time Series Analysis*, volume 4. Cambridge university press, 2000.

Jonas Peters, Joris M Mooij, Dominik Janzing, and Bernhard Schölkopf. Causal discovery with continuous additive noise models. *Journal of Machine Learning Research*, 2014.

Jonas Peters, Dominik Janzing, and Bernhard Schlkopf. *Elements of Causal Inference: Foundations and Learning Algorithms*. The MIT Press, 2017a. ISBN 0262037319.

Jonas Peters, Dominik Janzing, and Bernhard Schölkopf. *Elements of causal inference: foundations and learning algorithms*. The MIT Press, 2017b.

Yinghua Ren, Wanru Zhao, Wanhai You, and Kaikai Zhai. Multiscale and partial correlation networks analysis of risk connectedness in global equity markets. *Physica A: Statistical Mechanics and its Applications*, 573:125911, 2021.

Jakob Runge, Sebastian Bathiany, Erik Bollt, Gustau Camps-Valls, Dim Coumou, Ethan Deyle, Clark Glymour, Marlene Kretschmer, Miguel D Mahecha, Jordi Muñoz-Marí, et al. Inferring causation from time series in Earth system sciences. *Nature communications*, 10(1):1–13, 2019.

Thilo A Schmitt, Desislava Chetalova, Rudi Schäfer, and Thomas Guhr. Non-stationarity in financial time series: Generic features and tail behavior. *EPL (Europhysics Letters)*, 103(5):58003, 2013.

Bernhard Schölkopf, Francesco Locatello, Stefan Bauer, Nan Rosemary Ke, Nal Kalchbrenner, Anirudh Goyal, and Yoshua Bengio. Toward causal representation learning. *Proceedings of the IEEE*, 109(5): 612–634, 2021.

Gideon Schwarz. Estimating the dimension of a model. *The Annals of Statistics*, pp. 461–464, 1978.

Yanning Shen, Brian Baingana, and Georgios B Giannakis. Nonlinear structural vector autoregressive models for inferring effective brain network connectivity. *arXiv preprint arXiv:1610.06551*, 2016.

Shohei Shimizu, Patrik O. Hoyer, Aapo Hyvärinen, and Antti Kerminen. A linear non-Gaussian acyclic model for causal discovery. *Journal of Machine Learning Research*, 7:2003–2030, December 2006. ISSN 1532-4435.

Shohei Shimizu, Takanori Inazumi, Yasuhiro Sogawa, Aapo Hyvärinen, Yoshinobu Kawahara, Takashi Washio, Patrik O. Hoyer, and Kenneth Bollen. Directlingam: A direct method for learning a linear non-gaussian structural equation model. *Journal of Machine Learning Research*, 12:1225–1248, July 2011. ISSN 1532-4435.

Christopher A Sims. Macroeconomics and reality. *Econometrica: Journal of the Econometric Society*, pp. 1–48, 1980.

Peter Spirtes, Clark N Glymour, Richard Scheines, and David Heckerman. *Causation, Prediction, and Search*. MIT press, 2000.

Matthew J Vowels, Necati Cihan Camgoz, and Richard Bowden. D'ya like DAGs? A survey on structure learning and causal discovery. *ACM Computing Surveys*, 55(4):1–36, 2022.

Gang-Jin Wang, Chi Xie, Min Lin, and H Eugene Stanley. Stock market contagion during the global financial crisis: A multiscale approach. *Finance Research Letters*, 22:163–168, 2017.

Junfeng Yang and Xiaoming Yuan. Linearized augmented Lagrangian and alternating direction methods for nuclear norm minimization. *Mathematics of computation*, 82(281):301–329, 2013.

Xing Yang, Chen Zhang, and Baihua Zheng. Segment-wise time-varying dynamic Bayesian network with graph regularization. *ACM Transactions on Knowledge Discovery from Data (TKDD)*, 16(6):1–23, 2022.

Yue Yu, Jie Chen, Tian Gao, and Mo Yu. DAG-GNN: DAG structure learning with graph neural networks. In *International Conference on Machine Learning*, pp. 7154–7163. PMLR, 2019.

Xun Zheng, Bryon Aragam, Pradeep Ravikumar, and Eric P Xing. DAGs with no tears: Continuous optimization for structure learning. In *Advances in neural information processing systems*, volume 31, 2018.

Xun Zheng, Chen Dan, Bryon Aragam, Pradeep Ravikumar, and Eric Xing. Learning sparse nonparametric DAGs. In *International Conference on Artificial Intelligence and Statistics*, pp. 3414–3425. PMLR, 2020.

Shengyu Zhu, Ignavier Ng, and Zhitang Chen. Causal discovery with reinforcement learning. In *International Conference on Learning Representations*, 2020.

Appendix A   Comparison with DYNOTEARS

Figure 7 depicts the swarm plot concerning the number of edges and the SHD (structural Hamming distance) of the estimated matrices of causal coefficients. The latter metric indicates the number of modifications needed to retrieve the ground truth from the estimated causal graph (the lower, the better). First, we observe that both models converge to causal networks of similar size. In addition, by looking at SHD, we notice that dagness function linearization does not cause a worsening in estimation accuracy.

(a) $\mathbf{W}^0$

(b) $\mathbf{W}^1$

Figure 7: Swarm plots regarding the number of edges (left) and SHD (right) of the estimated causal matrices.

(a) $\mathbf{W}^0$

(b) $\mathbf{W}^1$

Figure 8: Swarm plots regarding the building blocks of SHD (from the left: extra, missing and reverse edges wrt the ground truth) associated with the estimated causal matrices $\mathbf{W}^0$ (a) and $\mathbf{W}^1$ (b). Please notice that in case of lagged causal interactions, we cannot observe reverse edges.

The comparison in terms of accuracy between DYNOTEARS and SS-CASTLE is further detailed below. In particular, Figure 8 shows the contribution of *extra*, *missing* and *reverse* edges to the SHD. More precisely:

- *extra edges* are estimated edges not encompassed in the causal graph skeleton;

- *missing edges* are causal connections present in the ground truth that have not been retrieved, neither with a wrong direction;
- *reverse edges* are those connection estimated with a wrong direction.

We observe that the number of missing edges is by far the most dominant component (especially in case of larger networks). Overall, the models perform similarly across the three components. It is worth noticing that, since $\mathbf{W}^1$ is acyclic by definition, we cannot have reverse edges.

Appendix B Hyper-parameters

The table below provides the chosen values for λ during the experimental assessment of SS-CASTLE.

| Nodes | p | λ | | |
		T=100	T=500	T=1000
	1.0	0.50	0.10	0.10
	1.5	0.10	0.05	0.05
10	2.0	0.50	0.10	0.10
	2.5	0.10	0.05	0.01
	100.0	0.10	0.05	0.01
	1.0	0.50	0.10	0.10
	1.5	0.10	0.05	0.05
30	2.0	0.50	0.10	0.10
	2.5	0.10	0.05	0.01
	100.0	0.10	0.05	0.01
	1.0	0.50	0.10	0.10
	1.5	0.50	0.05	0.05
50	2.0	0.50	0.10	0.10
	2.5	0.10	0.05	0.05
	100.0	0.10	0.05	0.01

Table 1: Selected values for λ for each of the considered parameters combinations $(T, N, p)_i$.

The table below shows the values of λ used in the experimental assessment of MS-CASTLE. In our experiments, we considered $\lambda \in \{0.0001, 0.0005, 0.001, 0.005, 0.01, 0.05, 0.1, 0.5\}$.

Nodes	p	Transform	λ T=128	T=512	T=8192
5	1.0	None	0.0100	0.0050	0.0050
		swt-db3	0.0500	0.0100	0.0100
		swt-db5	0.0500	0.0100	0.0100
		swt-db7	0.0500	0.0100	0.0100
	2.0	None	0.0050	0.0050	0.0010
		swt-db3	0.0050	0.0010	0.0010
		swt-db5	0.0050	0.0010	0.0001
		swt-db7	0.0050	0.0010	0.0005
10	1.0	None	0.0500	0.0100	0.0050
		swt-db3	0.0500	0.0100	0.0100
		swt-db5	0.0500	0.0500	0.0100
		swt-db7	0.0500	0.0500	0.0100
	2.0	None	0.0050	0.0010	0.0010
		swt-db3	0.0100	0.0050	0.0010
		swt-db5	0.0100	0.0050	0.0010
		swt-db7	0.0100	0.0050	0.0010
30	1.0	None	0.1000	0.0100	0.010
		swt-db3	0.0500	0.0500	0.0100
		swt-db5	0.0500	0.0500	0.0100
		swt-db7	0.0500	0.0500	0.0500
	2.0	None	0.0500	0.0050	0.0005
		swt-db3	0.0100	0.0050	0.0005
		swt-db5	0.0100	0.0050	0.0010
		swt-db7	0.0100	0.0050	0.0010

Table 2: Selected values for λ for the tested versions of MS-CASTLE, as indicated by the column *Transform*.

Appendix C   Additional Comparison with non-Gaussian Methods

Sensitivity to data set size.

Figure 9 provides additional details concerning the structural mistakes made by the models. In particular, we provide the comparison with VAR-DirectLiNGAM and VAR-ICALiNGAM in terms of SHD, and its building blocks, i.e., extra, missing and reverse edges. Overall, SS-CASTLE outperforms the baselines also in terms of the considered structural metrics. Looking at the instantaneous causal interactions (top rows), we notice how non-Gaussian methods tend to estimate a greater number of extra and reverse edges, even when $T = 1000$. With regards to missing edges, all the models tend to perform similarly as T grows. Again, the results show that non-Gaussian methods display a dependence on the value of p. In order to better interpret the values of SHD, consider that in case $N = 30$ and $s = .85$, on average only 65 entries of $\mathbf{W}^0$ are different from zero due to the acyclicity requirement.

Concerning lagged causal interactions (bottom rows). We see that the non-Gaussian methods are prone to return solutions characterized by a large number of extra edges. Regarding SS-CASTLE, the number of missing edges turns out to be the major contributor to SHD in case of small data sets ($T = 100$). With the increase of T, extra and missing edges start to contribute similarly to the aforementioned structural metric.

Sensitivity to network size.

Figure 10 provides further information regarding the estimated structure when we vary the network size. Also in this case we see that SS-CASTLE outperforms the considered baselines. Concerning the learning of the matrix of instantaneous relations, we see that non-Gaussian methods are prone to estimate a greater number of extra and reverse edges. With regards SS-CASTLE, the main component of SHD is the number

Figure 9: Comparison with VAR-DirectLiNGAM and with VAR-ICALiNGAM in the estimation of the causal matrices $\mathbf{W}^0$ (top) and $\mathbf{W}^1$ (bottom) in terms of a SHD, and its building blocks, i.e., b extra edges, c missing edges, and d reverse edges. Each subfigure depicts the case when $N = 30$ and the number of time series N varies in $\{100, 500, 1000\}$.

Figure 10: Comparison with VAR-DirectLiNGAM and with VAR-ICALiNGAM in the estimation of the causal matrices $\mathbf{W}^0$ (top) and $\mathbf{W}^1$ (bottom) in terms of a SHD, and its building blocks, i.e., b extra edges, c missing edges, and d reverse edges. Each subfigure depicts the case when $T = 1000$ and the number of time series N varies in $\{10, 30, 50\}$.

of missing edges. As far as the learning of the matrix of lagged causal interactions, the results show that, even though the models display a similar number of missing arcs, overall SS-CASTLE is more robust to extra edges.

Appendix D Multiscale Causal Structure

The multiscale causal structure determining the data generated for the experimental assessment of MS-CASTLE consists of 4 different time scales. In addition to instantaneous causal interactions, to test also the performance of MS-CASTLE in the presence of lagged interactions, we set the autoregressive lag $L = 1$, for each time scale.

In detail, over the first time scale $\mathbf{W}_0^1$ has entries $[\mathbf{W}_0^1]_{i,i+1} = 0.6$ and zero elsewhere, $i \in [N-1]$; $\mathbf{W}_1^1$ has entries (i) $[\mathbf{W}_1^1]_{i,i} = -0.6$, with $i \in [N]$, (ii) $[\mathbf{W}_1^1]_{j,j+1} = 0.3$, with $j \in [N-1]$, (iii) $[\mathbf{W}_1^1]_{k+1,k} = 0.3$, with $k \in [N-1]$, and (iv) zero elsewhere.

At the second scale $\mathbf{W}_0^2$ has entries $[\mathbf{W}_0^2]_{i+2,i} = -0.5$, with $i \in [N-2]$, and zero elsewhere; $\mathbf{W}_1^2$ has entries (i) $[\mathbf{W}_1^2]_{i,i} = -0.5$, with $i \in [N]$, (ii) $[\mathbf{W}_1^2]_{j,j+2} = 0.4$, with $j \in [N-2]$, (iii) $[\mathbf{W}_1^2]_{k+2,k} = -0.4$, with $k \in [N-2]$, and (iv) zero elsewhere.

Over the third and fourth scale we set $\mathbf{W}_1^3$ with entries (i) $[\mathbf{W}_1^3]_{i,i} = 0.5$, with $i \in [N]$, (ii) $[\mathbf{W}_1^3]_{j,j+1} = -0.4$, with $j \in [N-1]$, (iii) $[\mathbf{W}_1^3]_{k+1,k} = 0.4$, with $k \in [N-1]$, and (iv) zero elsewhere; $\mathbf{W}_1^4$ with entries (i) $[\mathbf{W}_1^4]_{i,i} = -0.7$, with $i \in [N]$, and zero elsewhere.

Finally, in our experiments, we consider $N \in \{5, 10, 30\}$.

Appendix E MS-CASTLE: Additional Results on Synthetic Data

Figure 11: Comparison of different versions of MS-CASTLE in terms of normalized SHD (i.e., SHD divided by the number of edges in the ground truth), obtained in the experimental settings described in Section 4.3.1. Subplots on the top refer to the Gaussian setting, whereas those on the bottom to the non-Gaussian one. Subplots on the left refer to the case $N = 5$, those on the center to $N = 10$, and those on the right to $N = 30$. Dashed lines represent the inter-quartile range.

Appendix F Financial Data

We consider data concerning 15 global equity markets at daily frequency. To focus on covid-19 pandemic period, we restrict our attention to observations from January 2020, the 2nd to April 2021, the 30th. In our analysis, we deal with the following markets: *All Ordinaries Index* (AOR, Australia), *Hang Seng Index* (HSI, Hong Kong), *Nikkei 225 Index* (NKX, Japan), *Shanghai Composite Index* (SHC, Shanghai), *Straits Times*

Figure 12: Behavior of equity markets during the considered period. All indexes are rebased to 100.

Index (STI, Singapore), *TAIEX Index* (TWSE, Taiwan), *DAX Index* (DAX, Germany), *FTSE MIB Index* (FMIB, Italy), *IBEX Index* (IBEX, Spain), *CAC 40 Index* (CAC, France), *FTSE 100 Index* (UKX, UK), *RTS Index* (RTS, Russia), *Bovespa Index* (BVP, Brazil), *Nasdaq Composite Index* (NDQ, US), *S&P/TSX Composite Index* (TSX, Canada). The data has been downloaded from Stooq[2]. Figure 12 depicts the behavior of the indexes during the considered time window. In particular, the indexes plummet during the first months of 2020 and, subsequently, they show a second downturn during October 2020. In addition, Table 3 provides summary statistics. Overall, according to risk adjusted return[3], Sortino ratio[4] and average compounded return to max drawdown ratio (ACR/MDD), TWSE and NDQ outperform the rest of the indexes. Moreover, we see that annualized average compounded returns largely vary across the considered instruments: while IBEX and UKX are the worst performing, TWSE and NDQ are the most profitable. Furthermore, all indexes show a high level of volatility. Among the others, BVP and RTS are the most volatile indexes. Last but not least, all indexes suffer heavy losses during the analysed period, as shown by max drawdown metric (MDD). Interestingly, SHC shows the lowest value.

	AOR	HSI	NKX	SHC	STI	TWSE	DAX	FMIB	IBEX	CAC	UKX	RTS	BVP	NDQ	TSX
Avg Comp. Ret. (%)	3.57	2.12	15.79	8.40	-1.30	28.29	10.08	1.15	-9.33	1.88	-7.43	-5.60	2.15	31.41	7.76
Volatility (%)	25.94	22.32	23.65	19.26	21.07	19.74	29.25	31.12	30.36	28.79	26.24	36.12	39.69	32.46	29.00
Risk Adj. Ret. (%)	0.14	0.10	0.67	0.44	-0.06	1.43	0.34	0.04	-0.31	0.07	-0.28	-0.16	0.05	0.97	0.27
Sortino (%)	0.18	0.13	0.99	0.60	-0.08	2.03	0.47	0.05	-0.41	0.09	-0.37	-0.20	0.07	1.34	0.35
MDD (%)	37.09	25.33	31.27	14.62	31.93	28.72	38.78	41.54	39.43	38.56	34.93	49.46	46.82	30.12	37.43
ACR/MDD	0.10	0.08	0.50	0.57	-0.04	0.98	0.26	0.03	-0.24	0.05	-0.21	-0.11	0.05	1.04	0.21
Skew	-1.10	-0.37	0.27	-0.76	-0.44	-0.54	-0.63	-2.26	-1.05	-0.96	-0.80	-1.02	-1.04	-0.69	-1.01
Kurtosis	7.37	1.87	5.01	6.49	7.22	5.40	10.27	20.19	11.14	9.49	8.94	7.01	11.32	7.35	18.77
1st %-ile (%)	-6.16	-4.18	-4.47	-3.60	-4.63	-3.94	-5.00	-5.21	-4.69	-5.38	-4.03	-7.12	-9.37	-5.16	-6.76
5th %-ile (%)	-2.33	-2.28	-2.16	-1.86	-1.75	-1.80	-3.38	-2.81	-2.95	-3.00	-2.79	-3.35	-3.21	-3.12	-2.12
Min	-9.52	-5.56	-6.08	-7.72	-7.35	-5.83	-12.24	-16.92	-14.06	-12.28	-10.87	-13.02	-14.78	-12.32	-12.34
Max	6.56	5.05	8.04	5.71	6.07	6.37	10.98	8.93	8.57	8.39	9.05	9.23	13.91	9.35	11.96

Table 3: Summary statistics of equity markets at daily frequency. Average compounded return, volatility, risk adjusted return, and Sortino Ratio are annualised.

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[2]The website is reachable at `https://stooq.pl/`.

[3]The risk adjusted return is a performance metric, defined as average compounded return to volatility ratio.

[4]Sortino ratio evaluates risk adjusted performance of a financial instrument discounting for its downside standard deviation.

To get the series of markets risk, as measured by conditional volatility, we model the logarithmic returns of indexes by means of GARCH models (Bollerslev, 1986). We use the latter econometric technique to measure systemic risk of equity markets while capturing stylized facts of equity returns, such as volatility clustering (i.e., large (small) swings in stock prices tend to group together), heteroscedasticity (i.e., time-dependent variance) and fat-tailedness (i.e., kurtosis greater than 3). With regards to GARCH parameters, we select the best combination according to lowest value of BIC criterion (Schwarz, 1978).

Appendix G   Additional Results Concerning the Causal Analysis of the Risk of Global Equity Markets

Figure 13: Highly persistent causal matrices (top) and corresponding SSCGs (bottom) for three different values of $\bar{c}$. Red entries in the causal matrices represent positive coefficients, whereas blue ones are negative. With regards to the SSGS, green nodes are American stock indexes, pink the European ones, and purple the Asian.

Figure 14: Highly persistent multiscale causal matrix for three different values of $\bar{c}$. Red entries in the causal matrices represent positive coefficients, whereas blue ones are negative.

Figure 15: Highly persistent MSCG for three different values of $\bar{c}$. With regards to the SSGS, green nodes are American stock indexes, pink the European ones, and purple the Asian.