Department of Mathematics and Computer Science
Statistics Group

Structure Learning in Multiple Time Series

Master Thesis

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Abstract

This is the abstract.

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Preface

This Master's Thesis contains the work . This thesis has been written to complete two Master's studies at the Eindhoven University of Technology. The Master "Computer Science and Engineering" with a specialization in "Data Sciene in Engineering", as well as the Master "Industrial Applied Mathematics" and symbolizes the completion of both Master's studies.

I would like to acknowledge my dr. Rui Castro for his supervision and guidance throughout this final project. Rui has helped greatly in shaping the project from the very beginning, and providing different perspectives and directions throughout the final project. Whenever hurdles arose in the journey, Rui helped me in either getting over these hurdles, or circumvent them alltogether.

Furthermore, I would like to acknowledge my appreciation to dr. Alex Mey for his valuable input into the project as well. His feedback and insightful perspectives have been of great value to me during this final project.

Lastly, I would also like to thank my colleagues, friends and family for keeping me motivated not just during this final year, but throughout my entire academic career. They provided the necessary distraction next to my Master's thesis.

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List of Definitions

$A \otimes B$ - The *Kronecker product* of two matrices $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{p \times q}$. Performing this operation yields an $mp \times nq$ matrix.

I_n - The *identity matrix* with dimensions $n \times n$.

n - Total number of samples per variable.

p - Total number of nodes in a graph; Total number of variables in a dataset; Number of time series in our dataset.

P_{DS} - A *doubly stochastic matrix.* A matrix $P_{DS} \in \mathbb{R}^{p \times p}$ is doubly stochastic if and only if both all its rows as its columns sum to one. More specifically,

$$\sum_{i=1}^{p} p_{ij} = \sum_{j=1}^{p} p_{ij} = 1 \qquad \forall i, j = 1, \cdots, p.$$

P_{perm} - A *permutation matrix.* A matrix $P_{perm} \in \{0,1\}^{p \times p}$ is a permutation matrix if and only if both all of its rows and columns contain exactly one non-zero entry. This only non-zero entry must be equal to one.

T - Number of time steps in a time series.

$\mathrm{Tr}(A)$ - The *Trace* of a square matrix $A \in \mathbb{R}^{p \times p}$ is defined to be the sum of its diagonal entries. More specifically,

$$\mathrm{Tr}(A) = \sum_{i=1}^{p} A_{ii}.$$

$vec(A)$ - The *vectorization operation* applied on a matrix $A \in \mathbb{R}^{m \times n}$. This operation transforms the matrix A by stacking the n columns of $A_{\cdot,i}, i = 1, \cdots, n$ on top of each other. More specifically,

$$vec(A) = (a_{11}, a_{21}, \cdots, a_{m1}, a_{12}, \cdots, a_{m2}, \cdots, a_{1n}, \cdots, a_{mn})^T.$$

$X_{t,i}$ - The value of time series i at time step t.

$X_{\cdot,i}$ - The ith *time series*, often of dimension T, the number of time steps. When there is no ambiguity possible, we might use the notation $X_{\cdot,i} \equiv X_i$.

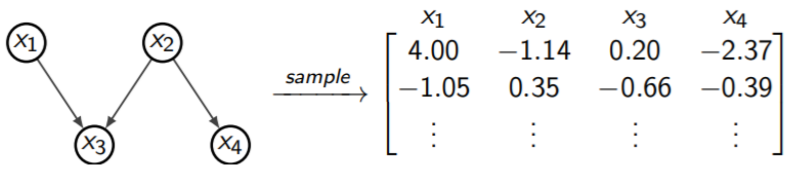
$X_{t,\cdot}$ - The p dimensional vector $\{X_{t,1}, \ldots, X_{t,p}\}$, containing the data values of our p time series. When there is no ambiguity possible, we might use the notation $X_{t,\cdot} \equiv X_t$.

$\mathbf{X}$ - The *data matrix*, often a subset of $\mathbb{R}^{T \times p}$, consisting of p time series of length T.

Chapter 1

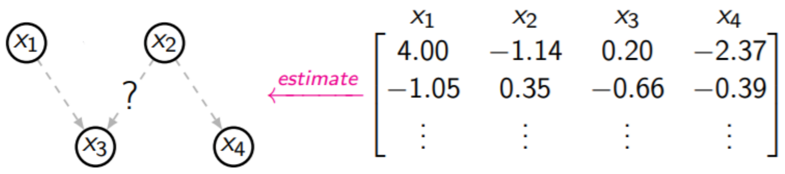
Introduction

This thesis explores the interesting domain of *structure learning*. In many scenarios, we have a graphical model, and we take *samples* generated by this graphical model. This process of sampling is depicted in Figure 1.1. In structure learning, the focus is on the opposite direction. Given a set of samples, the goal is to infer the structure of the graphical model that generated these samples. In other words, were are interested in learning the structure of the graphical model that generated our samples. This process of structure learning is depicted in Figure 1.2.



$$\begin{array}{cccc} x_1 & x_2 & x_3 & x_4 \\ \left[\begin{array}{cccc} 4.00 & -1.14 & 0.20 & -2.37 \\ -1.05 & 0.35 & -0.66 & -0.39 \\ \vdots & \vdots & \vdots & \vdots \end{array}\right] \end{array}$$

Figure 1.1: Visualization of *sampling* data from a graphical model [16].



$$\begin{array}{cccc} x_1 & x_2 & x_3 & x_4 \\ \left[\begin{array}{cccc} 4.00 & -1.14 & 0.20 & -2.37 \\ -1.05 & 0.35 & -0.66 & -0.39 \\ \vdots & \vdots & \vdots & \vdots \end{array}\right] \end{array}$$

Figure 1.2: Visualization of *estimating* the structure of a graphical model from data [16].

Applications. Structure learning is an important concept that with many applications, predominantly concerning complex systems. In a world where systems are becoming evermore complex, it is important to have a suitable graphical model that captures its behavior. Nowadays, systems are so complex that they defy human intuition.

An example of a system so complex that it defies our intuition are genetic regulatory systems. Through these systems, we can understand which genes are expressed where in the organism, and to which extent. Most of these genetic regulatory systems involve many interlocking positive and negative feedback loops, making these systems so complex that they defy human intuition. More information on such complex networks in gene regulatory systems can be found in [9].

Apart from complex biological systems, even man-made systems can become so complex that they will defy human intuition. Based on human knowledge alone, it is not guaranteed that a man-made complex system will perfectly adhere to this intended structure. Furthermore, these man-made systems have become so complex that it is impossible for one person to comprehend its complete behavior. Examples of such complex machines are abundant throughout the tech industry, such as the EUV lithography systems manufactured by ASML.

Therefore, we see that there is a need for *data driven* approaches to construct models for these systems. The approaches will be particularly effective in the era of big data, where data through measurements in genetic regulatory systems or through sensors in man-made machines is widely available.

Motivation. Having seen some interesting applications for structure learning, let us now consider the benefits of having learned the structure of such a complex system. Consider a large and complex machine with many interacting components. When the machine breaks, it might be so complex that finding the issue can take a long time and require disassembling the machine completely. By using sensors, it is possible to know that something has gone wrong in the machine. However, this can be uninformative. The fact that a sensor reports anomalous values does not imply that the root cause is anywhere near this sensor. This is where structure learning comes into play. Suppose that we have analyzed the sensors of the working machine for a long enough period of time. If we can learn the structure of these sensors, very important information can be retrieved from this structure. First of all, whenever the machine breaks, we can look at which sensors produce anomalous results. Indeed, the most logical approach is still to first inspect the components around these sensors. However, if the issue does not lie there, we can use our learned structure to propose other components that are likely to be the root cause of the problem. Therefore, structure learning can be very useful for *root cause analysis* in complex systems.

Another advantage of using structure learning for complex machines is that we can verify whether indeed in theory non-interacting components indeed have no interaction in practice. If we can physically decompose the machine into multiple sections, each with their own function, the learned structure should adhere to this physical structure as well. Should this not be the case, then we know that something went wrong in either design or manufacturing process. Hence, structure learning can be a useful tool for *system validation* as well.

Objective. The objective throughout this thesis is to develop data driven approaches that can learn the structure of complex systems. More precisely, we are interested in learning *predictive causal networks.* The learned network describes the directed causal relations in between the nodes. Note that with causal relations we merely mean predictive causality, in other words, whether the values corresponding to one node are helpful in predicting another node. A visualization of the objective is given in Figure 1.2.

Outline. This thesis is structured as follows. In Chapter 3, important definitions and notions are introduced that are deemed necessary to read through this thesis. In Chapter 4, we will discuss several existing methods for structure learning. These existing methods range from a variety of different techniques, and hence all have their niche in the current state of the art literature. In Chapter 5, we will introduce novel methods that we have researched during this thesis. Our methods will be benchmarked against the aforementioned methods in Chapter.

Chapter 2

Problem Setting

Data notation

Consider the setting where we observe $p \in \mathbb{N}$ continuous variables over a duration of time $T \in \mathbb{N}$. We denote these variables by our *data matrix*

$$\mathbf{X} \in \mathbb{R}^{p \times T}.$$

Here, T can be seen as our time horizon. At each time step $t = 1, \dots, T$, we observe our p variables, yielding real-valued measurements $X_{t,1}, X_{t,2}, \dots, X_{t,p}$. Let $X_{t,\cdot} \in \mathbb{R}^p$ denote the p dimensional vector of measurements of our p variables at a specific time t. Furthermore, let $X_{\cdot,i} \in \mathbb{R}^T$ denote the T measurements of variable $i = 1, \dots, p$, ordered from $t = 1$ until $t = T$. We also denote by $X_{\cdot,i}$ the ith time series in our data matrix $\mathbf{X}$, and $\{X_{\cdot 1}, \dots, X_{\cdot,p}\}$ the set of our p time series. When there is no ambiguity possible, the notations $X_t \equiv X_{t,\cdot}$ and $X_i \equiv X_{\cdot,i}$ might be utilized to ease notation.

We assume that this data matrix $\mathbf{X}$ has been generated by some joint distribution $p(\mathbf{X})$. However, this joint distribution is unknown, and all that is available to determine this joint distribution is our data matrix $\mathbf{X}$. The goal is partly to recover this joint distribution $p(\mathbf{X})$, but we are predominantly interested in the graphical model that corresponds to this distribution $p(\mathbf{X})$. The next paragraph will explain what this graphical model will look like.

Graph representation

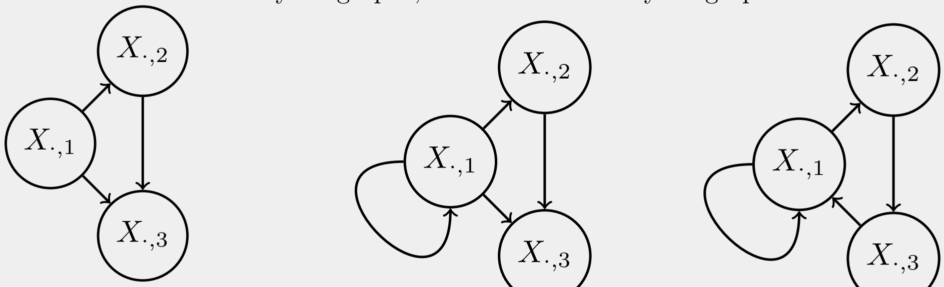
Given our data matrix $\mathbf{X}$, let us consider the directed graph representation $G(\mathbf{X}) = (V, A)$ consisting of p vertices. So, $|V| = p$, and the set of arcs or directed edges is $A = \{(x, y) \mid x, y \in V\}$. Vertex i refers to , $X_{\cdot,i}$, the ith time series in our data matrix. Therefore, a directed edge (i, j) indicates a directed relationship from $X_{\cdot,i}$ to $X_{\cdot,j}$. In the context of this thesis, such a directed edge implies a *directed predictive power*. In other words, the variable or time series $X_{\cdot,i}$ is helpful in predicting $X_{\cdot j}$. When there is no edge (i, j), both variables do not seem helpful in predicting each other. We say that $X_{\cdot,i}$ and $X_{\cdot,j}$ are conditionally independent.

We can also denote our directed edge set A as an *adjacency matrix* $A \in \{0, 1\}^{p \times p}$, where an entry A_{ij} is equal to one if there is an directed edge (i, j), and zero otherwise. In mathematical notation,

$$A_{ij} = \begin{cases} 1 & \text{if } (i, j) \in A, \\ 0 & \text{otherwise.} \end{cases}$$

The goal of this thesis is to build such a directed graph $G(\mathbf{X}) = (V, A)$ based on our data matrix $\mathbf{X}$, under one extra constraint. The directed graph $G(\mathbf{X})$ must be *acyclic*. Nevertheless, our definition of acyclic deviates slightly from the literature. Given that our data matrix consists of p time series, it is not unlikely that a time series $X_{\cdot,i}$ will be helpful in predicting itself. Therefore, we do allow for *self-loops*, which are cycle of length 1. Therefore, when we say that $G(\mathbf{X})$ must be acyclic, we require that it does not contain any cycle of length *greater* than 1. We call such a directed acyclic graph a DAG for short throughout this thesis. Three examples that explain what we consider to be a directed acyclic graph are given in Example 2.1.

Example 2.1 Two directed acyclic graphs, and one directed cyclic graph.



(a) The graph G_a. (b) The graph G_b. (c) The graph G_c.

Figure 2.1: Three different graphs with $p = 3$ vertices. G_a consists of three edges $(1, 2)$, $(1, 3)$, and $(2, 3)$. As it does not contain any cycles, G_a is a DAG. G_b consists of the same edges, but now a self-loop $(1, 1)$ is added. G_b is not a DAG in the standard graph theory literature, as it contains a cycle of length 1. As mentioned before, we allow for cycles of length 1 and therefore, we consider G_b to be a DAG throughout this thesis. G_c consists of the same edges as G_b, but the edge $(1, 3)$ is flipped, resulting in the edge edge $(3, 1)$. Consequently, G_c contains a cycle of length 3 now, which we do not consider to be a DAG.

Furthermore, we also want to quantify the predictive power in the edge (i, j). Rather than simply stating whether there is a directed edge (i, j) or not, we want to assign a weight $w(i, j)$ as well to this edge. This weight quantifies the *strength* of the edge (i, j). We assign such a weight to all directed edges (i, j). Therefore, we will end up with a *weighted* adjacency matrix W, which is equal to

$$W_{ij} = \begin{cases} w(i,j) \cdot A_{ij} & \text{if } A_{ij} = 1, \\ 0 & \text{otherwise.} \end{cases}$$

We use the abbreviation WAM for the weighted adjacency matrix. An example of a graph induced by such a WAM is given in Example 2.2. The goal of this thesis is not only to determine the underlying DAG, but also determine the weights of the directed edges. The problem can therefore informally be stated as follows:

Given $\mathbf{X}$, what is the "most suitable" WAM W such that $G(\mathbf{X})$ is a DAG (self-loops allowed)?

Note that the "most suitable" is put between quotes to indicate that this is certainly not a mathematically sound formulation. The elaboration on "most suitable" will come later in this chapter.

Example 2.2 The graph $G(W_b)$.

Consider the graph G_b depicted in Figure 2.1 (b). Its adjacency matrix is given in Equation 2.1. Furthermore, suppose that we assign weights to each edge, so that we are given the weighted adjacency matrix that is also given in Equation 2.1:

$$A_b = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \qquad W_b = \begin{pmatrix} 0.5 & 0.3 & 0.2 \\ 0 & 0 & 0.8 \\ 0 & 0 & 0 \end{pmatrix}. \tag{2.1}$$

Then, a visualization representation of the graph G_b with the weighted adjacency matrix W_b is given in Figure 2.2.

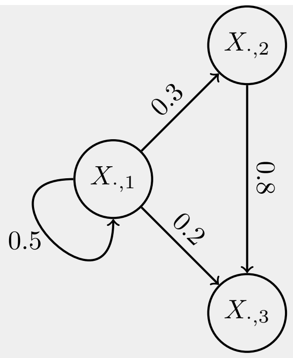


Figure 2.2: The weighted graph $G_b(W_b)$ from Figure 2.1 (b), where the weighted adjacency matrix W_b is given in Equation 2.1.

Difficulties

Having given a first explanation of the problem at hand, let us first discuss some difficulties that have already arisen. Learning the directed acyclic structure of $\mathbf{X}$ is quite challenging for multiple reasons.

First of all, when a variable $X_{\cdot,i}$ is useful in predicting $X_{\cdot,j}$, the converse could be true as well. Hence, $X_{\cdot,j}$ could also be useful in predicting $X_{\cdot,i}$. However, our graph $G(\mathbf{X})$ cannot contain cycles of length greater than 1, so it cannot contain both arcs. Therefore, we need not only know whether $X_{\cdot,i}$ is useful in predicting $X_{\cdot,j}$, but also whether $X_{\cdot,i}$ is *more* useful in predicting $X_{\cdot,i}$ than vice versa. In other words, apart from detecting whether there is a dependency between two variables, we also need to determine the most suitable *directionality* of the dependency.

Secondly, the total number of possible DAGs grows super-exponentially with p, the number of time variables. In fact, when we have only ten variables, the total number of possible DAGs already is a staggering $4.2 \cdot 10^{18}$ [12]. In other words, the search space of our problem is super-exponential. Hence, simply trying all possible directed acyclic graphs is not a tractable solution. Furthermore, we have not even discussed yet how to find a suitable WAM W given this adjacency matrix A. In fact, Chickering et al. has shown that the problem at hand is NP-hard [7], meaning that it is highly unlikely for a method to exist that will solve this problem exactly in polynomial time. In the current literature, algorithms that can solve this problem exactly are only tractable for tens of time series.

Formal Problem Statement. Let us concretize the problem statement further. We have explained what we are looking for, but what remains unclear is what the "most suitable" W is for our data matrix $\mathbf{X}$. This had been left blank before is because there is no universally best choice of W. There are many different *cost functions* that can be used to determine whether a choice of W is "good". For now, we abstract from the cost function, and denote this by $C(W)$, to indicate that the only parameter we optimize over is the weighted adjacency matrix W. Now, we define the "most suitable" W as a matrix that minimizes the given cost function $C(W)$. Therefore, the overarching goal of this thesis is to find

$$W^* = \operatorname*{arg\,min}_{W \in \mathbb{R}^{p \times p}} C(W) \text{ such that } G(W) \text{ is a DAG (self loops allowed).}$$

Lastly, we need to define what cost function $C(W)$ we will use. This will be done in the next paragraph, as there exist multiple suitable cost functions.

Cost functions $C(W)$ In order to determine whether a weighted adjacency matrix W is a good fit for our data matrix $\mathbf{X}$, we need some sort of cost function $C(W)$ that quantifies the goodness of fit. Therefore, let us consider some possible cost functions.

The first possibility of a valid cost function is the *negative log likelihood function* of the data $\mathbf{X}$. The likelihood function described the likelihood of the data $\mathbf{X}$ being generated by some statistical model. The joint distribution $\hat{p}(W;\mathbf{X})$ associated with this statistical model this can be described by a set of parameters, in our scenario a matrix W. We can optimize this joint distribution with respect to W. The larger $p(W;\mathbf{X})$, the more likely the data matrix $\mathbf{X}$ has been generated by the statistical model parametrized by W. Hence, we want to maximize $p(W;\mathbf{X})$ with respect to W. Equivalently, we can minimize the negative log-likelihood, which is obtained by taking the natural logarithm of $p(W;\mathbf{X})$, and changing the sign:

$$\ell(W;\mathbf{X}) = -\ln\left(p\left(W;\mathbf{X}\right)\right).$$

A second possibility is also known as the mean squared error (MSE), which is the average of the sum of squared residual errors. In the literature, it is also known as the L_2 loss function. Three equivalent notations are

$$\begin{aligned} MSE(\hat{\mathbf{X}};\mathbf{X}) &= \frac{1}{T}\|\mathbf{X}-\hat{\mathbf{X}}\|_F^2 && (2.2)\\ &= \frac{1}{T}\sum_{t=1}^{T}\left\|X_{\cdot,t}-\hat{X}_{\cdot,t}\right\|_2^2 && (2.3)\\ &= \frac{1}{T}\sum_{t=1}^{T}\sum_{i=1}^{p}\left(X_{i,t}-\hat{X}_{i,t}\right)^2. && (2.4)\end{aligned}$$

where $\hat{\mathbf{X}}$ is our estimate of the data matrix $\mathbf{X}$. Analogously, $\hat{X}_{\cdot,t}$ is our estimate for $X_{\cdot,t}$, and $\hat{X}_{i,t}$ is our estimate for $X_{i,t}$.

Another possibility is the mean absolute error (MAE), which is the average of the sum of the residuals in absolute value. Another name for the mean absolute error is L_1 loss. The formula for the mean absolute error is

$$\begin{aligned} \text{MAE}(\hat{\mathbf{X}};\mathbf{X}) &= \frac{1}{T}\sum_{t=1}^{T}\|X_{\cdot,t}-\hat{X}_{\cdot,t}\|_1 && (2.5)\\ &= \frac{1}{T}\sum_{t=1}^{T}\sum_{i=1}^{p}\left|X_{i,t}-\hat{X}_{i,t}\right|. && (2.6)\end{aligned}$$

Regularization An extra feature that we prefer our weighted adjacency matrix W to have is that it is *sparse*. This means that we want W to achieve a small loss and at the same time, we prefer for W to have few non-zero entries. This is often achieved by adding regularization. Adding an L_1 regularization penalty to the weighted adjacency matrix W. In mathematical notation, this means that we add an L_1 penalization with respect to W, $\rho(W)$, which is defined as

$$\rho(W) = \lambda\|W\|_1 := \lambda\left(\sum_{i=1}^{p}\sum_{j=1}^{p}|W_{ij}|\right),$$

where $\lambda \geq 0$ determines how strong the penalty will be for having non-zero entries.

Let us now define our objective more formally. When we say we are looking for the "most suitable" weighted adjacency matrix W, we mean that this W minimizes some cost function $C(W)$. This cost function can be any sensible combination of the loss functions and regularization techniques mentioned above. For now, we stick to the following cost function:

$$C(W,\lambda) = MSE(\hat{\mathbf{X}};\mathbf{X}) + \lambda\|W\|_1. \tag{2.7}$$

In Equation 2.7, We have omitted the dependency of our cost function on $\mathbf{X}$, as we can not optimize the cost function over a fixed data matrix $\mathbf{X}$. Note that we do not have $\mathbf{X}$ as a parameter of our cost function, as our estimator $\hat{\mathbf{X}}$ will be parametrized by the weighted adjacency matrix W.

Estimating the data matrix $\hat{\mathbf{X}}$ Since we have defined our cost functions in the previous paragraph, the new variable $\hat{\mathbf{X}}$ has appeared, which is the *estimator* for our data matrix $\mathbf{X}$. In this paragraph, we will explain which model we will use to estimate our data. For this, we use a vector autoregressive model of order 1, or VAR(1) for short. Our estimator is defined as

$$\hat{X}_{t,\cdot} = X_{t-1,\cdot}W, \qquad t = 2, ..., T \tag{2.8}$$

where $X_{t-1,\cdot} \in \mathbb{R}^p$ are the actual values of the previous timestep, and $W \in \mathbb{R}^{p\times p}$ is our weighted adjacency matrix. We see that we have no estimator for the first time step, as we have no previous time step. Therefore, the mean squared error is equal to

$$\begin{aligned} MSE(\hat{\mathbf{X}}; \mathbf{X}) &= \frac{1}{T-1}\sum_{t=2}^{T} \|X_t - X_{t-1}W\|_2^2 \\ &= \frac{1}{T-1}\left\|\mathbf{X}_{[2:T]} - \mathbf{X}_{[1:T-1]}W\right\|_F^2. \end{aligned}$$

From Equation 2.8, we see that our estimator $\hat{X}_{t,i}$ is in fact a linear combination of the p time series at time step $t-1$. Therefore, we can only expect our estimator to capture linear relations. Furthermore, we can only expect our estimator to capture from one time step ago. This restricts our estimator quite heavily. However, the simplicity yields a clear graphical model, namely a single directed acyclic graph. This is an unavoidable trade-off; the more complex we make our estimator $\hat{\mathbf{X}}$, the more complex it is to describe the relations between the time series.

To conclude the problem setting, consider the data matrix $\mathbf{X} \in \mathbb{R}^{T\times p}$. Given this data matrix, we are interested in capturing the directed relations between these p time series. The collection of these directed relations is captured in a weighted adjacency matrix W of a graph $G(W)$ on p nodes, one node for each time series. We constrain this collection of relations W by requiring $G(W)$ to be a directed acyclic graph with self-loops allowed. We consider W^* to be the weighted adjacency matrix that optimally captures the relationships, where we define optimally to be

$$W^* = \underset{\substack{W\in\mathbb{R}^{p\times p},\\ G(W)\text{ a DAG.}}}{\arg\min} \frac{1}{T-1}\|\mathbf{X}_{[2:T]} - \mathbf{X}_{[1:T-1]}W\|_F^2. \tag{2.9}$$

Therefore, we can conclude this chapter with the formal notation of our problem setting:

$$\text{Given } \mathbf{X}\text{, find } W^* = \underset{\substack{W\in\mathbb{R}^{p\times p},\\ G(W)\text{ a DAG.}}}{\arg\min} \frac{1}{T-1}\sum_{t=2}^{T}\|X_t - X_{t-1}W\|_2^2 + \lambda\|W\|_1.$$

The next chapter will discuss some of the existing literature that focuses on solving variants of this problem.

Chapter 3

Preliminaries

3.1 Graph Theory

Graph.

Directed Acyclic Graph.

3.2 Models

3.2.1 Vector AutoRegression Model

A Vector AutoRegressive (VAR) model

$$X_t = \sum_{i=1}^{p} A_i X_{t-i} + e$$

3.2.2 Structural Equation Model

$$X = AX + e$$

3.2.3 Structural Vector AutoRegression Model

A Structural Vector AutoRegression Model (SVAR) model consists of both a SEM and a VAR part. We can write this as

$$X = AX + \sum_{p=1}^{p} A_i X_{t-1} + e.$$

Chapter 4

Previous Work

- *Exact methods:* These methods will find an exact solution to the problem. However, their running time will be exponential. These methods are only tractable for at most a dozen variables.
- *Approximate methods:* Given that exact methods are only applicable to a doze nodes, we need to accept a trade-off: methods that can are much faster than exponential, however, they can not guarantee the best solution. So, these methods could for example be applied to hundreds of nodes, but they cannot guarantee that the solution it finds is anywhere near the optimal solution.

4.1 Exact methods

4.1.1 GOBLNIP

4.1.2 Dynamic Programming

4.2 Approximate methods

4.2.1 NOTEARS

NOTEARS (*Non-combinatorial Optimization via Trace Exponential and Augmented lagRangian for Structure learning*) is a method developed by Zheng et al [15] from the Carnegie Mellon University. As in this thesis, the topic of interest is structure learning: inferring a directed acyclic graph from data. The authors focus on a linear Structural Equation Model of the form

$$X = WX + z.$$

The most difficult hurdle to overcome is the combinatorial constraint that the inferred structure must be a directed acyclic graph. In their paper, they present a novel strategy. Rather than solving the (partly) combinatorial optimization problem, they translate it to an equivalent continuous optimization problem.

$$\begin{array}{rl} \min\limits_{W \in \mathbb{R}^{d\times d}} & F(W) \\ \text{subject to} & G(W) \in \mathsf{DAGs} \end{array} \quad \iff \quad \begin{array}{rl} \min\limits_{W \in \mathbb{R}^{d\times d}} & F(W) \\ \text{subject to} & h(W) = 0, \end{array} \tag{4.1}$$

Now, the function $F(\cdot)$ that the authors try to optimize is the least-squares loss plus an ℓ_1 regularization on the weighted adjacency matrix to encourage sparsity of the DAG. In mathematical notation, this is equal to

$$F(W) = \frac{1}{2n} \|\mathbf{X} - \mathbf{X}W\|_F^2 + \lambda \|W\|_1.$$

The continuous function that enforces acyclicity is

$$h(W) = \operatorname{Tr}\left(e^{(W \circ W)}\right) - d.$$

Here $W \circ W$ represents the *Hadamard product* of two matrixes. In other words, it is the element-wise square of the matrix W. The authors note four reasons for choosing this function as $h(W)$. First of all, $h(W) = 0$ if and only if W represents the weighted adjacency matrix of a DAG, and the value of $h(W)$ represents the "DAG"ness of W. Furthermore, the function as well as its gradient are smooth and can also be easily evaluated.

Optimization The authors use the *augmented Lagrangian* method to solve the right-hand side of Equation 4.1. To solve the augmented Lagrangian, an iterative two-step procedure is proposed. This pseudocode for this procedure is given in Algorithm 1. First, we optimize the augmented Lagrangian with respect to W (Line 3 of Algorithm 1). Secondly, we optimize the augmented Lagrangian with respect to the Lagrange multiplier α (Line 4 of Algorithm 1). The augmented Lagrangian with a penalty parameter $\rho > 0$ and a Lagrange multiplier α can be written as

$$L^{\rho}(W, \alpha) = F(W) + \frac{\rho}{2}|h(W)|^2 + \alpha h(W). \tag{4.2}$$

Equation 4.2 can be solved using a dual ascent method with respect to W and α. The dual function with the Lagrange multiplier α is given by

$$D(\alpha) = \min_{W \in \mathbb{R}^{d \times d}} L^{\rho}(W, \alpha). \tag{4.3}$$

To optimize Equation 4.3, the authors use the L-BFGS-B optimization method [17]. They used the implementation in the Python package `scipy` [1, 2, 13]. Now that we have found a local minimizer W_{α}^{*} of Equation 4.3, the next step is to find a local solution to the dual problem

$$\max_{\alpha \in \mathbb{R}} \; D(\alpha). \tag{4.4}$$

Luckily, $D(\alpha)$ is linear with respect to alpha, and its derivative is simply $\nabla D(\alpha) = h(W_{\alpha}^{*})$. The authors propose to simply do one step of dual gradient ascent with step size ρ. The dual gradient ascent is given by the formula

$$\alpha_{t+1} = \alpha_t + \rho \nabla D(\alpha). \tag{4.5}$$

The algorithm that the authors propose is an iterative procedure of two steps. First, optimize the augmented Lagrangian with respect to W using the L-BFGS-B optimization method. Secondly, optimize the augmented Lagrangian with respect to the Lagrange multiplier α using Equation 4.5. This iterative procedure is continued until a matrix W_{ECP} is found such that $h(W)$ is sufficiently small (Line 5 of Algorithm 1). This is the solution of the equality-constrained program (ECP), the right-hand side of 4.1.

The final part of the algorithm is *thresholding*. This means that all entries of W_{ECP} that are smaller than some threshold ω will be set to zero. Thresholding reduce the number of false positives []. Furthermore, as this algorithm is a numerical procedure, there will be inevitably some numerical precision errors near machine precision, so setting a threshold of for example $\omega = 10^{-8}$ would solve that issue as well. Experiments done by the authors also demonstrate that thresholding increases the accuracy in structure learning.

To conclude, the approach described in NOTEARS is a fundamentally novel approach that transforms the combinatorial constraint $G(W) \in \mathsf{DAGs}$ into a continuous constraint $h(W) = 0$. Then using a quite simple iterative two-step procedure using the augmented Lagrangian method, a local minimum could be found using existing solvers. Note that only a local minimum is guaranteed, and not a global minimum, as the search space is non-convex. Given that the problem at hand is NP-hard, this comes as no surprise. Should this method always find a global minimum, then an algorithm would exists that solves an NP-hard problem in polynomial time, which has never been found before.

Algorithm 1 NOTEARS

```
1: Input: Initial guess $(W_0, \alpha_0)$, progress rate $c \in (0,1)$, tolerance $\epsilon > 0$, threshold $\omega > 0$.
2: while F door $t = 0, 1, 2, \ldots$:
3:     Solve primal $W_{t+1} \leftarrow \arg\min_W L^\rho(W, \alpha_t)$ with $\rho$ such that $h(W_{t+1}) < ch(W_t)$.
4:     Dual ascent $\alpha_{t+1} \leftarrow \alpha_t + \rho h(W_{t+1})$.
5:     If $h(W_{t+1}) < \epsilon$, set $\tilde{W_{\mathsf{ECP}}} = W_{t+1}$ and break.
6: end while
7: Return the thresholded matrix $\widehat{W} := \tilde{W_{\mathsf{ECP}}} \circ 1(|\tilde{W_{\mathsf{ECP}}}| > \omega)$.
```

However, the fact that only a local minimum is guaranteed does not seem to be a detrimental problem. The authors have compared the local optimum found using Algorithm 4.1 to the global optimum found using an exact program. In this scenario, the authors have used the GOBNILP program to find the global minimum. Quite often, the local optimum was close to the global optimum, which demonstrates that the non-convexity is not a large issue.

4.2.2 Relaxing to the Birkhoff Polytope

The paper *Learning Bayesian Networks through Birkhoff Polytope: A Relaxation Method* by Dallakyan et al. [8] describes a method that is similar to our research direction. The authors assume a linear structural equation model (SEM), which is of the form

$$X = BX + \varepsilon,$$

where $\varepsilon = (\varepsilon_1, \cdots, \varepsilon_p)^T$, $\varepsilon_j \sim \mathcal{N}\left(0, \omega_j^2\right), j = 1, \cdots, p$. We denote B to be the *weighted adjacency matrix*, and $\Omega = \text{diag}(w_1^2, \cdots, w_p^2)$ to be the *inverse covariance matrix*. This weighted adjacency matrix B defines the structure of the underlying directed acyclic graph $\mathcal{G}$. A non-zero entry b_{ij} represents an edge from variable X_j to variable X_i in $\mathcal{G}$.

The distribution of X, where X adheres to a linear SEM, is well known, namely

$$X \sim \mathcal{N}_p(\mathbf{0}, (I - B)^T \Omega^{-1} (I - B).$$

The negative log-likelihood of can be written as

$$\begin{aligned} l(B, \Omega \mid \mathbf{X}) &= \frac{1}{2} \text{Tr}\left(\mathbf{X}^T \mathbf{X} (I - B) \Omega^{-1} (I - B)\right) + \frac{n}{2} \log |\Omega| \\ &= \frac{1}{2} \text{Tr}\left(P \underbrace{\mathbf{X}^T \mathbf{X}}_{=nS} P^T \underbrace{(I - B_\pi) \Omega_\pi^{-T/2}}_{=L^T} \underbrace{\Omega_\pi^{-1/2} (I - B_\pi)}_{=L} \right) - n \log \underbrace{|\Omega_\pi|^{-1/2}}_{=|L| = \prod_{j=1}^p L_{jj}} \\ &= \frac{1}{2} \text{Tr}\left(PSP^T L^T L)\right) - \sum_{j=1}^p \log L_{jj} \\ &=: l(L, P|\mathbf{X}) \end{aligned}$$

An important note to make is that $l(L, P|\mathbf{X})$ is *permutation invariant*, in other words,

$$l(L, P|\mathbf{X}) = l(L, I|\mathbf{X}) \ \forall \text{ permutation matrices } P.$$

To overcome this permutation invariance, the authors use the same approach as []. They regularize such that sparse DAGs are more preferred by adding a minimax concave penalty (MCP) $\rho(\cdot)$. This MCP is applied to all lower triangular entries of L. The final non-convex penalized score function that the authors consider is

$$Q(L, P) = \min_{L, P} \left(l(L, P|\mathbf{X}) + \sum_{1 \le j \le i \le p} \rho\left(|L_{ij}|; \lambda\right) \right).$$

In order to optimize , the authors propose an iterative approach; first optimize P, then optimize L. This is done until we have a maximum number of iterations k_{max} has been reached.

Algorithm 2 RRCF algorithm

```
1: input:
2: $\lambda, k_{max} \leftarrow$ Tuning Parameter, iteration
3: $L^{(0)}, P^{(0)} \leftarrow$ Initial matrices
4: while $k < k_{max}$:
5:     $\hat{P}^{(k)} = \arg\min_{P \in \mathcal{P}_p} Q_{RRCF}(L^{(k-1)}, P)$
6:     $\hat{L}^{(k)} = \arg\min_{L \in \mathcal{L}_p} Q_{RRCF}(L, P^{(k)})$
7:     $k = k + 1$
8: Output: $(\hat{L}, \hat{P})$
```

To optimize P (line 5 of Algorithm 2), the authors relax the constraints from the set of permutation matrices to the set of doubly stochastic matrices. If we only omit the terms that are constant in with respect to P, then we get that we need to minimize.

However,

To optimize L (line 6 of Algorithm 2), the authors propose a cyclic coordinatewise algorithm.

Algorithm 3 Cholesky Factor Estimation

```
1: input:
2: $k_{max}, \mathbf{X}, \lambda, \gamma, \epsilon$
3: $L^{(0)} \leftarrow$ Initial Cholesky factor
4: For i = 1,2,..., p
5:   $\beta^i = \arg\min_{\beta_i} Q_{RRCF,i}(\beta^i)$  via Algorithm
6: Construct $L \in \mathcal{L}_p$ by setting its non-zero values as $\beta^i$
7: Output: Lower diagonal matrix L
```

They have compared their method, which they have coined the Relaxed Regularized Cholesky Factor (RRCF) Framework, to three other existing methods; ARCS, CCDr, and NOTEARS. In the experiments, RRCF achieved results compatitble with these other methods.

However, the RRCF Framework suffers from some drawbacks. First of all, three tuning parameters, , need to be tuned. This can be computationally expensive, especially for high-dimensional datasets.

4.2.3 Using a genetic algorithm

The paper *Inferring large graphs using ℓ_1-penalized likelihood* by Champion et al. [6] proposes GADAG (*Genetic Algorithm for learning Directed Acyclic Graph*) to retrieve the underlying structure of a linear Gaussian Structural Equation Model, which is of the form

$$X = XG_0 + \varepsilon,$$

where $\varepsilon = (\varepsilon_1, \cdots, \varepsilon_p)^T$, $\varepsilon_j \sim \mathcal{N}\left(0, \sigma_j^2\right), j = 1, \cdots, p$. We denote G_0 to be the *weighted adjacency matrix.* This weighted adjacency matrix G_0 encodes the structure of the underlying directed acyclic graph $\mathcal{G}_0$. A non-zero entry g_{ij} represents an edge from variable X_i to variable X_j in $\mathcal{G}$.

To estimate this underlying graph G_0, the authors propose to use a penalized maximum likelihood method, which is of the form

$$\hat{G} = \arg\min\left(\ell(G) + \lambda \text{pen}\,(G)\right).$$

Omitting terms that are constant with respect to our variables, we get the following

$$\hat{G} = \arg\min\left(\frac{1}{n}\|X(I-G)\|_F^2 + \lambda\|G\|\right).$$

$$\left(\hat{P}, \hat{T}\right) = \arg\min \left(\frac{1}{n} \left\| X(I - PTP^T) \right\|_F^2 + \lambda \left\| T \right\| \right).$$

Minimizing P

4.2.4 PC Algorithm

4.2.5 Greedy Equivalent Search

Chapter 5

Method

We will assume that our data has been generated by a VAR(1) model, which is defined as

$$X_{t+1} = X_t W + E, \tag{5.1}$$

where $E \sim \mathcal{N}(\mathbf{0}, \Sigma)$. The matrix E is the random Gaussian noise, and the matrix W is a coefficient matrix. Here, t as index represents the time step which ranges from $t = 1$ until some time horizon $t = T$. Note that a more standard notation would be to put the matrix on the left side of X_t, as in Equation 5.2:

$$X_{t+1} = W' X_t + E. \tag{5.2}$$

Nevertheless, both equations are equivalent for $W' = W^T$. However, the notation $X_t W$ is more easily interpretable from a graphical point of view.

For the sake of simplicity, we assume that our initial value $X_0 = \mathbf{0}$. Note, however, that we could have picked any finite p-dimensional value as initial value. Changing this would have only shifted our VAR(1) model, thereby only changing the mean of X_t to X_0.

The coefficient matrix W encodes the structure of our model. If an entry w_{ij} is equal to zero, that means that the variable $X_{i,t}$ has no influence in determining the value of the variable $X_{j,t}$ for any time t. However, if w_{ij} is in absolute value larger than zero, the variable $X_{i,t}$ is used in determining the value of the variable $X_{j,t}$. The larger w_{ij} in absolute value, the greater the influence of variable X_i on variable X_j.

We can visualize the coefficient matrix W as a graph $G(W)$. A non-zero entry w_{ij} indicates that there is an edge from X_i to X_j. This is the reason why we have opted for the notation of Equation 5.1 rather than the notation of Equation 5.2. Had we used the notation from Equation 5.2, then the corresponding weighted adjacency matrix would be W^T. From now on, let us denote $G(W)$ the weighted directed graph that is induced by the weighted adjacency matrix W.

The largest difficulty to overcome throughout this thesis is that the weighted adjacency matrix W must be such that $G(W)$ is a directed acyclic graph.

5.1 Decomposition of the Weighted Adjacency Matrix W

To constrain ourselves to matrices W such that the inferred DAG is acyclic, we recall this useful statement:

$$G(W) \text{ is a DAG} \iff \exists \text{ a permutation matrix P s.t. } P^T W P \text{ is upper triangular.}$$

An easy way to see this is that if $G(W)$ is a DAG, then there must be at least one one node i which does not have any incoming arcs. This node i will be the first entry in our permutation. Now, remove i and all its outgoing arcs from the graph, leaving us with a graph G'. We can iterate this process and find a new node j which does not have any incoming arcs in G'. After this iterative procedure, we have found a permutation P such that $P^T W P$ is upper triangular.

Although this might not be the most useful statement, a similar statement can be used in our advantage.

$G(W)$ is a DAG $\iff \exists$ an upper triangular matrix A, a permutation matrix P s.t. $P^TAP = W$.

We can prove this statement by construction. Let $G(W)$ be the graph induced by the weighted adjacency matrix W. As $G(W)$ is a DAG, we can decompose W using a permutation matrix P^TAP such that P^TAP is upper triangular. Denote $A = P^TWP$, then we can revert this by using the same permutation matrix P. Trivially, we have that $PAP^T = PP^TWPP^T = IWI = W$.

The main reason for choosing this decomposition is that we do not have to worry about explicitly requiring $G(W)$ to be acyclic. We have changed the formulation of our problem in such a way this constraint is implicitly required. As long as we require A to be lower triangular and P to be a permutation matrix, we have automatically satisfied the acyclicity constraint.

The decomposition removes the explicit requirement that W must be acyclic, however, other hurdles arise that need to be overcome. As in any mathematical problem, circumventing one issue will create another issue. The question that arises then is which issue is the "least worrying". A large amount of this thesis is dedicated to answering this question; what other issues do arise because of this composition?

One issue that still remains is the combinatorial search space of permutation matrices. Finding the most suitable permutation matrix P has now become the largest issue. For a total of p time series, there are $p!$ possible permutations and hence, $p!$ possible permutation matrices. This search space is exponential, meaning that an exhaustive search will not be feasible for a reasonably large number of time series. Nevertheless, the search space has been greatly reduced. Let $G(n)$ be the number of possible directed acyclic graphs with n nodes. The value of $G(n)$ is given by the recurrence

$$G(n) = \sum_{k=1}^{n} (-1)^{k+1} \binom{n}{k} 2^{k(n-k)} G(n-k),$$

which was first given by Robinson in [12]. Even for just ten nodes, the number of possible dags is equal to $G(10) \approx 4.2 \cdot 10^{18}$, a staggering number. However, there are "only" $10! \approx 3.6$ million different permutations. Hence, the combinatorial search space of permutation matrices is far smaller than the search space of directed acyclic graphs, albeit still exponential in size with respect to the number of variables.

Interestingly, during this thesis, two other papers were discovered that have used a similar decomposition. These two papers are mentioned and discussed in Subsection and Subsection . Given that two recent papers use a comparable strategy and consequently achieve results competitive with the current state of the art, there are mixed feelings. On one hand, it showcases the sensibility of the decomposition. On the other hand, it shows that the approach is not completely new.

5.1.1 Finding the lower triangular matrix A when the permutation is known.

We have established before that finding a matrix W that induced a DAG is an NP-hard problem. We have shown that we can decompose this matrix W into two parts: a lower triangular matrix A, and a permutation matrix P. Interestingly, the problem becomes quite easy to solve when we have either one of these two at our disposal.

Suppose that we know the permutation of the variables. That is, we are given a permutation of our variables that indicates the direction of the dependencies.

5.1.2 Finding the permutation when A is known.

Now, suppose that we are given the lower triangular matrix A.

5.2 Continuous Optimization Approaches

5.2.1 Relax the permutation matrix constraint

Nevertheless, the combinatorial nature of the search space poses some problems. Continuous optimization procedures are unsuitable for these types of problems, and therefore combinatorial approaches would be required. Therefore, we propose a method to alleviate ourselves from the combinatorial search space. We relax the search space from the set of permutation matrices to the convex hull of permutation matrices. This convex hull is also known as the *Birkhoff polytope*.

Model definition

Therefore, we assume the model

$$X_{t+1} = P^T T P X_t + E, \tag{5.3}$$

where P is a permutation matrix and T is a lower triangular matrix. We can easily circumvent the acyclity constraint by estimating solely the lower triangular entries of T along with a permutation matrix P.

Note that a special property of a permutation matrix P is that its inverse is equal to its tranpose, i.e., $P^T_{perm} = P^{-1}_{perm}$. For reasons that will become more obvious later on, let us rewrite Equation to

$$X_{t+1} = P^{-1} T P X_t + E. \tag{5.4}$$

We propose to use the L_2-norm as a cost function:

$$C(A, P) = \frac{1}{T-1} \sum_{t=1}^{T} \left\| X_t - \hat{X}_t \cdot \right\|_2^2 \tag{5.5}$$

Here, X_t are the actual values of the time series at time t, and $\hat{X}_t$ are the estimates of the time series. Under our model assumptions, the cost function boils down to

$$C(A, P) = \frac{1}{T-1} \sum_{t=1}^{T} \left\| X_t - P^{-1} A P X_{t-1} \cdot \right\|_2^2 \tag{5.6}$$

It is important to note some characteristics of our cost function here. First of all, the inverse of the matrix P makes Equation 5.7 a *non-convex* optimization problem.

Furthermore, the inverse of the matrix P can create serious non-singularity issues. When P is a permutation matrix, then P^{-1} is simply equal to P^T. However, the inverse of P is not defined always defined. For example, the matrix

$$P = \begin{pmatrix} 0.333 & 0.333 & 0.333 \\ 0.333 & 0.333 & 0.333 \\ 0.333 & 0.333 & 0.333 \end{pmatrix}$$

does not have an inverse, meaning that our cost function is not well defined for singular matrices.

Furthermore, even when the matrix is non-singular, we can still encounter issues. Let ε be an arbitrarily small number. Consider the matrix

$$P = \begin{pmatrix} 0.333 - \varepsilon & 0.333 + \varepsilon & 0.333 \\ 0.333 + \varepsilon & 0.333 - \varepsilon & 0.333 \\ 0.333 & 0.333 & 0.333 \end{pmatrix}.$$

This matrix is non-singular, as all the rows are linearly independent. However, from a numerical point of view, the matrix is numerically unstable. For $\varepsilon = 0.05$, the inverse of P is equal to

$$P^{-1} = \begin{pmatrix} 4.5e15 & 4.5e15 & -9.0e15 \\ 4.5e15 & 4.5e15 & -9.0e15 \\ -9.0e15 & -9.0e15 & 1.8e16 \end{pmatrix}.$$

This example illustrates the singularity problems that arise from our decomposition. Although we have relieved ourselves from the issues of the combinatorial search space of permutation matrices, we are now left with the singularity issues of P. We have traded our combinatorial constraint problem in for this singularity problem.

Population setting

Let us first analyze this model in the population setting. In this setting, we assume we have the entire population as data, meaning that we can take rather than having n samples, we have $n \to \infty$ samples.

Cost function In order to estimate these matrices A and P, we use an L_2-norm of the difference between the actual value $X_{t,val}$ and the predicted value $X_{t,pred}$. Assume the data has been generated by some (unknown) A^*, P^*, i.e.,

$$X_{t+1,val} = P^{*T} A^* P^* X_{t,val} + E,$$

where E again represents the added noise to our model. Now assume that we have our two estimated matrices A and P. The corresponding cost function in the population setting is equal to

$$C(P, A, P^*, A^*, E) = \mathbb{E}\left[\|X_{t,val} - X_{t,pred}\|_2^2\right] \tag{5.7}$$

Derivation of the cost function We can decompose this cost function to gain more insights into whether this model makes sense. The $2 - norm$ of a p dimensional variable $X \in ı$ is

$$\|X\|_2 = \sum_{i=1}^{p} \sqrt{|x_i|\|}.^2$$

Hence, we have that

$$\begin{aligned} C(P, A, P^*, A^*, E) &= \mathbb{E}\left[\|X_{t,val} - X_{t,pred}\|_2^2\right] \\ &= \mathbb{E}\left[\sum_{i=1}^{p} (X_{t,val,i} - X_{t,pred,i})^2\right] \\ &= \operatorname{Tr}\left(\mathbb{V}\left(X_{t,val} - X_{t,pred}\right)\right). \end{aligned} \tag{5.8}$$

So, we need to derive the covariance of $X_{t,val} - X_{t,pred}$. Recall that

$$X_{t+1,val} = \underbrace{P^{*-1} A^* P^*}_{=B^*} X_{t-1,val} + E, \qquad X_{t=1,pred} = \underbrace{P^{-1} A P}_{=B} X_{t,val}.$$

Hence,

$$\begin{aligned} \mathbb{V}\left(X_{t+1,val} - X_{t+1,pred}\right) &= \mathbb{V}\left(B^* X_{t,val} + E - B X_{t,val}\right) && \text{By Equation 5.4} \\ &= \mathbb{V}\left((B^* - B) X_{t,val} + E\right) && \text{Rearrange terms} \\ &= \mathbb{V}\left((B^* - B) X_{t,val}\right) + \mathbf{V}\left(E\right) && \text{By independence of } E \\ &= (B^* - B) \mathbf{V}(X_{t,val}) (B^* - B)^T + \Sigma. && \text{Take } B^* - B \text{ out of } \mathbb{V}(\cdot) \end{aligned} \tag{5.9}$$

What remains now is to derive the $\mathbf{V}\left(X_{t,val}\right)$.

Deriving V $(X_{t,val})$**.** As we assume that E is a Gaussian, we know that $X_{t,val}$ will be a Gaussian as well. Furthermore, as we assume Our data is stationary with mean of $\mathbf{0}$, we know that $X_{t,val} \sim \mathcal{N}(\mathbf{0}, \Sigma_X)$. Note that this unconditional distribution does not depend on t. What is left is to estimate Σ_X. From existing literature on variational autoregressive models, we can easily derive the covariance of X_t. From e.g., [], we know that

$$X_{t+1} = AX_t + E \iff vec(\Sigma_X) = \left(I_{n^2} - (A \otimes A)\right)^{-1} vec(\Sigma),$$

where $vec(\cdot)$ represents the *vectorization operation*, and $\otimes$ represents the *kronecker product*.

Example 5.1. To make this notation clearer, consider this two-dimensional example where

$$A = \begin{pmatrix} 0.5 & 0 \\ 0.3 & 0.4 \end{pmatrix}, \qquad \Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}.$$

Performing the kronecker product $A \otimes A$ and subtracting that from I_{n^2} yields

$$\begin{aligned} I_4 - (A \otimes A) &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0.5 \begin{pmatrix} 0.5 & 0 \\ 0.3 & 0.4 \end{pmatrix} & 0 \begin{pmatrix} 0.5 & 0 \\ 0.3 & 0.4 \end{pmatrix} \\ 0.3 \begin{pmatrix} 0.5 & 0 \\ 0.3 & 0.4 \end{pmatrix} & 0.4 \begin{pmatrix} 0.5 & 0 \\ 0.3 & 0.4 \end{pmatrix} \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0.25 & 0 & 0 & 0 \\ 0.15 & 0.2 & 0 & 0 \\ 0.15 & 0 & 0.2 & 0 \\ 0.09 & 0.12 & 0.12 & 0.16 \end{pmatrix} \\ &= \begin{pmatrix} 0.75 & 0 & 0 & 0 \\ -0.15 & 0.8 & 0 & 0 \\ -0.15 & 0 & 0.8 & 0 \\ -0.09 & -0.12 & -0.12 & 0.84 \end{pmatrix}. \end{aligned}$$

Then, calculating its inverse and multiplying it with the factorization of Σ yields

$$\begin{aligned} \left(I_n^2 - (A \otimes A)\right)^{-1} vec(\Sigma) &= \begin{pmatrix} 0.75 & 0 & 0 & 0 \\ -0.15 & 0.8 & 0 & 0 \\ -0.15 & 0 & 0.8 & 0 \\ -0.09 & -0.12 & -0.12 & 0.84 \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 2 \end{pmatrix} \\ &\approx \begin{pmatrix} 1.33 \\ 0.25 \\ 0.25 \\ 2.60 \end{pmatrix}. \end{aligned}$$

Therefore, we end this example by noting that the covariance of X_t is

$$\Sigma_X = \begin{pmatrix} 1.33 & 0.25 \\ 0.25 & 2.60 \end{pmatrix}.$$

Now, returning to deriving the value of $C(P, A, P^*, A^*, E)$ in the population setting, we have that

$$vec\left(\mathbb{V}\left(X_{t,val}\right)\right) = \left(I_{n^2} - B^* \otimes B^*\right)^{-1} vec(\Sigma).$$

Putting it all together We conclude that the expected cost function in the population setting equals

$$\begin{aligned} C(P, A, P^*, A^*, E) &= \operatorname{Tr}\left(\mathbb{V}\left(X_{t+1,val} - X_{t+1,pred}\right)\right) && \text{By Equation 5.8} \\ &= \operatorname{Tr}(\mathbb{V}((B^* - B)X_{t,val} + E) && \text{By Equation 5.9} \\ &= \operatorname{Tr}\left(\mathbb{V}((B^* - B)X_{t,val}) + \mathbf{V}(E)\right) && \text{By independence of } E \\ &= \operatorname{Tr}\left((B^* - B)\mathbb{V}(X_{t,val})(B^* - B)^T\right) + \operatorname{Tr}(\Sigma)\,. && \text{Take } B^* - B \text{ out} \end{aligned}$$

Global minimum of $C(A, P)$ Let us take a closer look at this cost function. The first question that arises is *what is the global minimum of this cost function?*. For this, we first remark that $\mathbb{V}(X_{t,val})$ is positive semi-definite. Furthermore, $\mathbf{V}(X_{t,val})$ is positive definite if it has full rank. Assuming our covariance is indeed full rank, we have that, for any B^*, B s.t. $B^* \neq B$,

$$(B^* - B)\mathbb{V}(X_{t,val})(B^* - B)^T > 0$$

and hence

$$C(P, A, P^*, A^*) = \operatorname{Tr}(\Sigma) \iff B^* = B.$$

In words, we can *only* attain the global minimum when we have exactly that our estimated matrix B is equal to the data generating matrix B^*.

This is a promising result for the population setting. We know that we can never attain a cost value smaller than the trace of Σ, and this value is only attained for A, P such that $P^{-1}AP = B^*$. Nevertheless, although there is only one global minimum with respect to B, there can still be many pairs of (A, P) to this specific value of B. Let us consider the scenario where

$$B^* = \begin{pmatrix} 0.5 & 0 & 0 \\ 0.3 & 0.4 & 0 \\ 0.2 & 0.0 & 0.6 \end{pmatrix}.$$

We only achieve our global minimum when $B = B^*$, but there are two pairs A_1, P_1 and A_2, P_2 that achieve this. The first pair is

$$A_1 = \begin{pmatrix} 0.5 & 0 & 0 \\ 0.3 & 0.4 & 0 \\ 0.2 & 0.0 & 0.6 \end{pmatrix}, P_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

and the second pair is

$$A_2 = \begin{pmatrix} 0.5 & 0 & 0 \\ 0.2 & 0.6 & 0 \\ 0.3 & 0.0 & 0.4 \end{pmatrix}, P_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

The reason for this is that there are multiple permutations possible, namely $(1, 2, 3)$ and $(1, 3, 2)$, as there is no dependence between our second and third variable. The fact that there are two ways to attain the global minimum is not a problem, however, as these are both compatible with the underlying graph and thus equally valid permutations.

A larger problem would be when the global minimum can also be achieved by a matrix P that is not a permutation matrix, but a doubly stochastic matrix. This would have problematic consequences, as the decoupling would make little sense then.

In short, an open question is, given a matrix $B^* = P^{-1}AP$, where P is a permutation matrix and A is a lower triangular matrix, does there exist a *doubly stochastic* matrix $\hat{P}_{DS}$ and a lower triangular matrix $\hat{A}$ such that $B^* = \hat{P}_{DS}^{-1}\hat{A}\hat{P}_{DS}$?. At the moment, the conjecture is that this is not the case, so the global optimum will only be reached using a valid permutation matrix P and a lower triangular matrix A.

Local minimum of $C(A, P)$ Now that we have seen that a global minimum of $C(A, P)$ indeed constitutes of a valid permutation matrix P and a lower triangular matrix A, the next question is whether there are any local optima that we can get stuck in. Given that our cost function is non-convex with respect to our matrix P, this suggests the presence of undesirable local optima. Furthermore, what is the nature of these local optima? Recall that a local optimum is where the gradient of the cost function is zero.

We indeed see that there are unpreferable local optima. Let us take a closer look at the nature of this local optimum. If we plot the cost functions and the gradients with respect to our entries in A, we see that the cost function is quadratic with respect to A, and hence the gradient is linear with respect to A. We see that all gradients are indeed zero for our values of A, indicating that it is indeed a local optimum with respect to A.

Let us now take a closer look at the cost function and the gradients with respect to our matrix P. As we can see, the matrix P is not a permutation matrix, but a doubly stochastic matrix. We already see that both the gradient and the cost function are not nice behaving functions. They have spikes which reach values up to $1e7$, meaning that the gradient is incredibly large for those values of p_{ij}. Another interesting thing we see is that most of the entries in p_{ij} are close to these spikes. Therefore, we see that the local optima occur where the doubly stochastic matrix P is very close to being non-singular. When inspecting the eigenvalues of P, we see that the first eigenvalue is equal to $-1e-3$, so being very close to zero. This is a major hurdle which is very difficult to overcome.

A solution that we would like to get is e.g. $A^* = B^*$, and P is the identity matrix. However, another global minimum exists as well, with

$$A =, P = .$$

Indeed, computing

Unfortunately, inferring the proper permutation matrix is the hardest part of this problem. For a total of p nodes, there are $p!$ permutations possible and therefore exponential in the number of nodes. The way we try to infer this is by *relaxing* the combinatorial constraint that P must be a permutation matrix. Instead of constraining P to be a permutation matrix, we only require P to be *doubly stochastic* matrix. In more precise words, we extend our search space from the set of permutation matrices to the Birkhoff polytope, the set of all doubly stochastic matrices. In this polytope, each of the vertices represents a matrix. Figure gives a visualization of the Birkhoff polytope for three dimensions.

We define the cost function to be

$$C(P, A, P^*, A^*, \Sigma^*) = \tag{5.10}$$

$$C(A, P, A^*, P^*) = \|X_{t,val} - X_{t,pred}\|_2^2 \,,$$

where we use the following value to predict X_t:

$$X_{t,pred} = P^{-1}APX_{t-1}$$

In reality, there is some underlying P^*, A^* used to generate $X_{t,val}$:

$$X_{t,val} = P^{*-1}A^*P^*X_{t-1} + \Sigma.$$

Gradient of the cost function

Now that the cost function has been derived and analysed, the next topic of interest is inferring P^* and A^*. One of the most straightforward methods to infer these parameters is by performing *gradient descent.* For this, we need to derive the partial derivatives of $C(P, A, P^*, A^*, E)$ with respect to its parameters. As only A and P here can be estimated, we write the cost function as $C(A, P)$. Let us first consider the gradient with respect to A.

Gradient of the cost function with respect to A. The gradient of $C(A, P)$ can be quite easily derived by using matrix derivatives. Furthermore, we know that computing the trace is a linear operation and thus, we can interchange the derivative and the trace.

$$\begin{aligned}
\frac{\partial C(P,A)}{\partial A_{ij}} &= \frac{\partial \mathrm{Tr}\left(\Sigma + (B^* - B)\,\Sigma_X\,(B^* - B)^T\right)}{\partial A_{ij}} && \text{(Fill in derived expected cost)}\\
&= \frac{\partial \mathrm{Tr}\,(\Sigma)}{\partial A_{ij}} + \frac{\partial \mathrm{Tr}\left((B^* - B)\,\Sigma_X\,(B^* - B)^T\right)}{\partial A_{ij}} && \text{(Separate sum of derivatives)}\\
&= \frac{\partial \mathrm{Tr}\,(\Sigma)}{\partial A_{ij}} + \mathrm{Tr}\left(\frac{\partial\,(B^* - B)\,\Sigma_X\,(B^* - B)^T}{\partial A_{ij}}\right) && \text{(Interchange trace and derivative)}\\
&= 0 + \mathrm{Tr}\left(\frac{\partial\,(B^* - B)\,\Sigma_X\,(B^* - B)^T}{\partial A_{ij}}\right) && \text{(Derivative of } \Sigma \text{ is 0)}\\
&= 2\mathrm{Tr}\left(\Sigma_X(B^* - B)^T\frac{\partial B^* - B}{\partial A_{ij}}\right) && \text{(Use chain rule)}\\
&= -2\mathrm{Tr}\left(\Sigma_X(B^* - B)^T P^{-1}J^{ij}P\right), && \text{(Work out last derivative)}
\end{aligned}$$

where

$$J^{ij}_{kl} = \begin{cases} 1 & k = i, l = j \\ 0 & \text{otherwise.} \end{cases}$$

In other words, J^{ij} is the matrix with zeros everywhere, except for the entry of the ith row and jth column, which is equal to one.

Gradient with respect to P Deriving the gradient of $C(A, P)$ with respect to P is slightly more involved than with respect to A, but nevertheless easily doable. Analogous to the gradient with respect to A, we first derive

$$\begin{aligned}
\frac{\partial C(P,A)]}{\partial P_{ij}} &= \frac{\partial \mathrm{Tr}\left(\Sigma + (B^* - B)\,\Sigma_X\,(B^* - B)^T\right)}{\partial P_{ij}} && \text{(Fill in derived expected cost)}\\
&= \frac{\partial \mathrm{Tr}\,(\Sigma)}{\partial P_{ij}} + \frac{\partial \mathrm{Tr}\left((B^* - B)\,\Sigma_X\,(B^* - B)^T\right)}{\partial P_{ij}} && \text{(Separate sum of derivatives)}\\
&= \frac{\partial \mathrm{Tr}\,(\Sigma)}{\partial P_{ij}} + \mathrm{Tr}\left(\frac{\partial\,(B^* - B)\,\Sigma_X\,(B^* - B)^T}{\partial P_{ij}}\right) && \text{(Interchange trace and derivative)}\\
&= 0 + \mathrm{Tr}\left(\frac{\partial\,(B^* - B)\,\Sigma_X\,(B^* - B)^T}{\partial P_{ij}}\right) && \text{(Derivative of } \Sigma \text{ is 0)}\\
&= 2\mathrm{Tr}\left(\Sigma_X(B^* - B)^T\frac{\partial B^* - B}{\partial P_{ij}}\right) && \text{(Use chain rule)}\\
&= -2\mathrm{Tr}\left(\Sigma_X(B^* - B)^T\left(-P^{-1}J^{ij}P^{-1}AP + P^{-1}AJ^{ij}\right)\right), && \text{(Work out last derivative)}
\end{aligned}$$

where

$$J^{ij}_{kl} = \begin{cases} 1 & k = i, l = j \\ 0 & \text{otherwise.} \end{cases}$$

To verify our derivations, we have plotted the

Inferring A and P

Now that we have a gradient for A and for P, we will describe multiple methods to infer A^* and P^*. A straightforward method to infer A^* in the population setting is as follows. We first estimate A^* without constraining A to be lower triangular. As we know that A^* is the weighted adjacency matrix of an actual directed acyclic graph, we know that there must exist at least one permutation matrix P_{perm} such that $A^* = PT^*P$, where T^* is lower triangular. Below, we give a straightforward algorithm to compute such valid permutation P.

Algorithm 4 Topological Sort

```
Input: A matrix $A$ that represents the weighted adjacency matrix of a directed acyclic graph.
Output: A permutation matrix $P$ that represents a valid topological ordering of the nodes of $G(A)$.
Set all diagonal entries of $A$ to zero.
while $A$ is nonempty do
    Let $i$ be the index of the row in $A$ with only zeros
    Remove this $i$th row from the matrix $A$
    Remove the $i$th column from the matrix $A$
end while
```

When A^* is the weighted adjacency matrix of a graph that is cyclic, which directed graph would then be the best solution? Is the problem even well-defined then?

Non-population setting

5.2.2 Using Birkhoff's Theorem

Another interesting method is by using Birkhoff's Theorem. Birkhoff's Theorem states the following.

Birkhoff's Theorem. Every doubly stochastic matrix can be rewritten as a *convex combination* of permutation matrices.

In more concrete words, let $P_1, P_2, \cdot, P_{n!}$ be all $n!$ possible permutation matrices. Given a doubly stochastic matrix P_{DS}, there exists non-negative $\lambda_1, ...\lambda_{n!} \in \mathbb{R}$, together summing to one, such that

$$P_{DS} = \sum_{i=1}^{n!} \lambda_i P_i.$$

This interesting result can be utilized in many different settings. Recall our model

$$X_{t+1} = P^{-1}APX_t.$$

Here, P is equal to a doubly stochastic matrix. Inferring these matrices A and P is quite difficult. Especially estimating a permutation matrix P is difficult given the combinatorial search space of all $n!$ permutation matrices. An interesting approach to circumvent this combinatorial search space is by relaxing the constraint from the set of permutation matrices to the set of doubly stochastic matrices. The second question then is how to deal with the new problems that arise when relaxing tho the space of doubly stochastic matrices. For example, the constraints that all entries must be between zero and one, and all rows must sum to one, and all columns must sum to one, require quite a large set of linear inequalities.

One way of dealing with this is by, instead of learning the entries of the douvly stochastic matrix directly, we learn the values λ_i, $i = 1, \cdots, n!$. So, we relax from requiring one specific permutation matrix to a convex combination of the existing permutation matrices. A problem, however, is that there are $n!$ permutation matrices, meaning that we now have a total of $\mathcal{O}(n!)$ permutations, which will not be feasible for large n. However, it is worth investigating this approach for moderately small n.

In more precise notation, let our cost function again by

$$\mathbb{E}\left[\|X_{val} - X_{pred}\|_2^2\right].$$

Then,

$$A, \{\lambda\}_{i=1}^{n!} = \arg \min_{A, \{\lambda\}_{i=1}^{n!}} \mathbb{E}\left[\|X_{val} - X_{pred}\|_2^2\right],$$

where

$$X_{val} = P^{*-1} A^* P^*,$$

and

$$X_{pred} = \left(\sum_{i=1}^{n!} \lambda_i P_i\right)^{-1} A \left(\sum_{i=1}^{n!} \lambda_i P_i\right).$$

5.2.3 As a product of row-swapping matrices

This method is similar to Subsection 5.1.3., "Using Birkhoff's Theorem". In that Subsection, we discussed the method of relaxing the space permutation matrix $\mathcal{P}_{perm}$ to the space of double stochastic matrices $\mathcal{P}_{DS}$. Consequently, we rewrote a double stochastic matrix $P_{DS} \in \mathcal{P}_{DS}$ as a convex combination of permutation matrices. Unfortunately, there are $n!$ permutation matrices and hence, an exponential number of parameters would have to be learnt and updated.

In this section, we discuss another method to relax the space of permutation matrices. For this, we define P_{ij} as the identity matrix with row i and row j swapped. As an example, consider three dimensions. Then, we have that

$$P_{13} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

Now, what is interesting, is that we can write any permutation matrix P as a product of $n-1$ of these row-swapping matrices. To see why this is the case, consider any permutation P. Let π be the ordering corresponding to the permutation matrix P, i.e., $\pi(i)$ contains the index of the row where the ith index is equal to 1. As an example, a permutation matrix P with corresponding order is

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \qquad \pi = (2, 3, 1).$$

Then, this permutation matrix P can be attained by only $n - 1 = 2$ row-swapping matrix multiplications, namely $P_{1,3}P_{2,3}$.

In the more general setting, we can always write any permutation matrix as a product of $n-1$ row-swapping matrices using a greedy approach. The first row-swapping matrix will swap the first row with the row of which the first index is equal to 1, so $P_{1,\pi(1)}$. The first row is now in the correct location. We continue with the subproblem of size $n-1$. The second row-swapping matrix will swap the second row with the row of which the second index is equal to 1, so $P_{2,\pi(2)}$. Clearly, we can do this iteratively until the first $n-1$ rows are in the correct location, which is after at most $n-1$ swaps. If the first $n-1$ rows are in the correct location, we can immediately deduce that the row with the nth index equal to 1 must be in the last row. Therefore, we can write any permutation matrix P as a product of $n-1$ row-swapping matrices.

Of course, these $n-1$ row-swapping matrices need not be the same for any permutation P. For one matrix, we swap row 1 and row 3, whereas for another matrix, we swap row 1 and row 2. Luckily, we know that we can write any matrix using $n-1$ row-swapping matrices, where we pick these from a total of $\binom{n-1}{2}$ matrices.

For the first swap, we can swap row 1 with any of the other $n-1$ rows, yielding $n-1$ possibilities. For the second swap, we swap row 2 with any of the remaining $n-2$ rows. This yields

$$\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} 1 = \sum_{i=1}^{n-1} n - i = \sum_{i=1}^{n-1} i = \frac{(n-1)(n)}{2} = \binom{n-1}{2}.$$

The main point here is that we can write a permutation matrix using only a linear number of row-swapping matrices, and the search space of all these matrices is quadratic. Therefore, the total number of parameters corresponding to this permutation matrix is significantly smaller than our approach involving Birkhoff's theorem, which yielded $n!$ parameters.

Now, let α_{ij} be a variable that is either zero or one, and it denotes whether we use this row-swapping matrix. By the convention we have that $P_{ij}^0 = I$, where I is the identity matrix. Furthermore, we have that $P_{ij}^1 = P_{ij}$.

Therefore, we can write any permutation matrix P as

$$P = \prod_{i=1}^{n-1} \prod_{j=i+1}^{n} P_{ij}^{\alpha_{ij}}, \qquad \alpha_{ij} \in \{0, 1\}.$$

Furthermore, the transpose or inverse is also easily calculated with respect to $P_{ij}^{\alpha_{ij}}$:

$$P^{-1} = \left(\prod_{i=1}^{n-1} \prod_{j=i+1}^{n} P_{ij}^{\alpha_{ij}} \right)^{-1} = \prod_{i=1}^{n-1} \prod_{j=i+1}^{n} \left(P_{ij}^{\alpha_{ij}}\right)^{-1} = \prod_{i=1}^{n-1} \prod_{j=i+1}^{n} \left(P_{ij}^{\alpha_{ij}}\right)^{T}.$$

Alternatively, another option is by reversing the order of the row-swapping matrices P_{ij}, so

$$P^{-1} = P^T = \left(\prod_{i=1}^{n-1} \prod_{j=i+1}^{n} P_{ij}^{\alpha_{ij}} \right)^{T}.$$

Relaxing α We see that we now have parametrized our permutation matrix P by the parameters $\alpha \in \{0,1\}^{\binom{n-1}{2}}$. However, learning these parameters is still not easy, as the α_{ij} are non-continuous. Therefore, we will try to relax this constraint by stating $\alpha_{ij} \in \mathbb{R}$. The hope is that relaxing this constraint means that we can use a continuous optimization procedure to learn our parameters α such as gradient descent. Let us see whether this is possible.

Let us first consider the matrix $P_{ij}^{\alpha_{ij}}$ for $\alpha_{ij} \in \mathbb{R}$. For $\alpha \in \mathbb{R}$, we have a *fractional matrix power*. The fractional matrix power with exponent $\alpha \in \mathbb{R}$ is defined as

$$A^{\alpha} = e^{\alpha \log(A)}$$

Eigendecomposition of P_{ij} Luckily, our matrices P_{ij} are all quite simple, only two rows are swapped. Therefore, let us consider the eigendecomposition of P_{ij}. We have that the eigenvalues of P_{ij} are

$$\lambda = \left(1, \ldots, 1, \underbrace{-1}_{\text{index } j}, 1, \ldots, 1 \right).$$

Furthermore, the corresponding eigenvector $\mathbf{u}_k$ of λ_k is equal to

$$\mathbf{u}_k = \begin{cases} e_k & \text{if } k \neq i \text{ and } k \neq j \\ \frac{1}{2}\sqrt{2}\,(e_i + e_j) & \text{if } k = i \\ \frac{1}{2}\sqrt{2}\,(e_i - e_j) & \text{if } k = j \end{cases},$$

where e_k denotes the vector with all zeros except a value one on the kth entry. Therefore, we can rewrite P_{ij} in its eigendecomposition

$$P_{ij} = U \Lambda U^T,$$

where U is the matrix with all eigenvectors stacked, and $\Lambda = \operatorname{diag}(\lambda)$.

Closed form of $P_{ij}^{\alpha_{ij}}$ Now, including the matrix exponent is quite easy when we have the eigendecomposition. We have that

$$P_{ij}^{\alpha_{ij}} = U\Lambda^{\alpha_{ij}}U^T.$$

As Λ is a diagonal matrix, its fractional matrix power can be computed by computing the power of all elements separately. As $n-1$ eigenvalues are equal to 1, we know that they remain the same, as $1^{\alpha_{ij}} = 1$ for any value of α_{ij}. Only for the eigenvalue with value -1, we interestingly get a value in the complex plane, as

$$-1^{\alpha_{ij}} = \cos(\pi\alpha_{ij}) + i\sin(\pi\alpha_{ij}).$$

We can put this all together to have a closed form solution for our matrix $P_{ij}^{\alpha_{ij}}$. Consequently, we also have a closed form solution for our matrix P, which is simply the product of all these matrices $P_{ij}^{\alpha_{ij}}$.

An important feature of $P_{ij}^{\alpha_{ij}}$ is that although its elements are complex numbers, $P_{ij}^{\alpha_{ij}}$ is still a doubly stochastic matrix for any value of α_{ij}, meaning that both its rows and columns sum up to 1 (and hence the imaginary part is equal to zero). Furthermore, we see that $P_{ij}^{\alpha_{ij}} = P_{ij}^{\alpha_{ij}+2k}$ for $k \in \mathbb{Z}$. Lastly, to compute its inverse, we can simply take the conjugate transpose of all matrices

$$P^{-1} = \left(\prod_{i=1}^{n-1}\prod_{j=i+1}^{n} P_{ij}^{\alpha_{ij}}\right)^{-1} = \prod_{i=1}^{n-1}\prod_{j=i+1}^{n} \left(P_{ij}^{\alpha_{ij}}\right)^{-1} = \prod_{i=1}^{n-1}\prod_{j=i+1}^{n} \left(P_{ij}^{\alpha_{ij}}\right)^{H}.$$

Alternatively, another option is by reversing the order of the row-swapping matrices $P_{ij}^{\alpha_{ij}}$ and taking their complex conjugates, so

$$P^{-1} = P^H = \left(\prod_{i=1}^{n-1}\prod_{j=i+1}^{n} \overline{P_{ij}^{\alpha_{ij}}}\right)^{T}.$$

Influence of α_{ij} on the cost value Now that we have a proper mathematical overview of how we can decompose this matrix P, let us consider how these α_{ij} will influence the cost function. Recall that throughout this thesis we will use the squared 2-norm of the residual error:

$$C(A, P) = \|X_{[1:T]} - X_{[0:T-1]}P^{-1}AP\|_2^2.$$

Let us denote

$$C(P) = \underset{A\text{lower triangular}}{\arg\min} \; C(A, P).$$

Given our permutation matrix P, we can easily derive this quantity using least squares. However, linear least squares will likely not work here as our P is not necessary a permutation matrix but a doubly stochastic matrix.

Nevertheless, we see that using certain values of α_{ij} can lead to a cost value smaller than the optimum of the original problem. This is problematic, as the optimum of the new problem does not coincide with the optimum of the old problem. Hence, this relaxation in its current form is not a good fit. A method to harshly penalize the complex part of the solution is necessary.

To see this, we start with a simple two-dimensional example, as then we only have one parameter α_{ij} and our permutation matrix is of the form

$$P = P_{12}^{\alpha}.$$

Let the true underlying weighted adjacency matrix be

$$W^* = \begin{pmatrix} 0.5 & 0 \\ 0.5 & 0.5 \end{pmatrix},$$

which corresponds to the permutation matrix P^* and lower triangular matrix A^*

$$P^* = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad A^* = \begin{pmatrix} 0.5 & 0 \\ 0.5 & 0.5 \end{pmatrix}.$$

Now, the α_{ij} that we hope to find would be $\alpha_{ij} = 0$, so that $P = P^*$. We sample $T = 50$ samples according to this model. This yields

$$C(A^*, P^*) \approx .$$

Now, what happens if we change our value of α? We have plotted the cost function $C(A^*, P_{12}^{\alpha})$. We see that the cost function behaves nicely with respect to α and the optimum is clearly at $\alpha = 0 + 2k, k \in \mathbb{Z}$. The reason for this is that $P_{ij}^{\alpha_{ij}}$ is cyclic with respect to α with a period of 2 (due to the cyclicty of $\cos(\pi\alpha) + i\sin(\alpha)$. Furthermore, we see that the cost function is symmetric around $\alpha = 1$. The reason for this symmetry is because

$$-1^{1+\alpha} = \cos(\pi + \pi\alpha) + i\sin(\pi + \pi\alpha) = \cos(\pi\alpha) - i\sin(\pi\alpha),$$

and hence

$$P_{ij}^{1+\alpha} = \overline{P_{ij}^{1-\alpha}}$$

. As the squared 2-norm of a complex number is equal for its complex conjugate, we see that

$$C\left(A, P_{ij}^{1+\alpha}\right) = C\left(A, P_{ij}^{1-\alpha}\right)$$

5.2.4 Learning using Lagrange Multipliers

As usual, we are interested in the following model:

$$X_{t+1} = P^{-1}APX_t + E$$

We have

$$C(A, P) = \mathrm{Tr}\left((B^* - B)\Sigma_X(B^* - B)\right),$$

where

$$B = P^{-1}AP.$$

Here, A is lower triangular and P is a doubly stochastic matrix, namely

$$\begin{aligned} 0 \le & p_{ij} & \forall\ i, j = 1, \cdots, n \\ \sum_{j=1}^{n} & p_{ij} = 1 & \forall\ i = 1, \cdots, n \\ \sum_{i=1}^{n} & p_{ij} = 1 & \forall\ j = 1, \cdots, n \end{aligned}$$

To deal with the $2n$ equality constraints, we use *lagrange multipliers* $\lambda_{row,i}$, $i = 1, \cdots, n$ and $\lambda_{col,j}$, $j = 1, \cdots, n$. The dual function now becomes

$$\mathcal{L}(A, P, \lambda) = C(A, P) - \sum_{i=1}^{n} \lambda_{row,i} \left(\sum_{j=1}^{n} p_{ij} - 1 \right) - \sum_{j=1}^{n} \lambda_{col,j} \left(\sum_{i=1}^{n} p_{ij} - 1 \right).$$

Let

$$q(\lambda) = \inf_{A,P} \mathcal{L}(A, P, \lambda).$$

Then the *dual problem* is

$$\max_{\lambda} q(\lambda).$$

To minimize $\mathcal{L}(A, P, \lambda)$, we will use gradient descent.

Gradient of $\mathcal{L}(A, P\lambda)$

The partial derivatives with respect to entries in A are simple,

$$\frac{\partial \mathcal{L}(A, P_\sigma, \lambda)}{\partial a_{ij}} = \frac{\partial C(A, P)}{\partial a_{ij}}$$

Now, the partial derivative with respect to the entries in p is more involved as it occurs also in exactly two equality constraints, namely in $\lambda_{row,i}$ and in $\lambda_{col,j}$.

$$\frac{\partial \mathcal{L}(A, P_\sigma, \lambda)}{\partial p_{ij}} = \frac{\partial C(A, P)}{\partial p_{ij}} - \lambda_{row,i} - \lambda_{col,j}.$$

Now, as $C(A, P)$ is unfortunately yet inevitably non-convex, we cannot expect to find the infimum $q(\lambda)$. However, let us consider a local minimum $\tilde{q}(\lambda)$, which we will find by gradient descent. Let us start with an initial matrix A_0 (e.g. the non-zero matrix) and an initial unconstrained matrix $P_0 = Z$, where $Z \sim \mathcal{N}(\mathbf{0}, I_{n^2})$.

For a sufficiently small step size, we will do this gradient descent until we have found a stationary point:

$$(A_{t+1}, P_{t+1}) = (A_t, P_t) - \eta \; \nabla \mathcal{L}(A_t, P_t, \lambda)$$

Note that this is an *unconstrained* optimization problem now, which should make things more easy.

Suppose that after a number of iterations, we have found this local minimum with parameters $\tilde{A}$, $\tilde{P}$. Then, we have that

$$\tilde{q}(\lambda) = \mathcal{L}(\tilde{A}, \tilde{P}, \lambda).$$

Now that we have $\tilde{q}(\lambda)$, the solution to the dual problem is

$$\max_\lambda \tilde{q}(\lambda),$$

which is again an unconstrained optimization problem, which we can also optimize by maximizing λ's.

$$\tilde{q}(\lambda) = C(\tilde{A}, \tilde{P}) - \sum_{i=1}^{n} \lambda_{row,i} \left(\sum_{j=1}^{n} \tilde{p}_{ij} - 1 \right) - \sum_{j=1}^{n} \lambda_{col,j} \left(\sum_{i=1}^{n} \tilde{p}_{ij} - 1 \right).$$

In order to maximize $\tilde{q}(\lambda)$ with respect to our lagrange multipliers, we note that $\tilde{q}(\lambda)$ is linear with respect to λ, meaning that

$$\frac{\tilde{q}(\lambda)}{\lambda_{row,i}} = \sum_{j=1}^{n} p_{ij} - 1,$$
$$\frac{\tilde{q}(\lambda)}{\lambda_{col,j}} = \sum_{i=1}^{n} p_{ij} - 1.$$

Unfortunately, these derivatives are constant and non-zero with respect to our lagrange multipliers. This means that there are no stationary points, and hence no local optima that we can hope to find using this approach. If a row or column i of our doubly stochastic matrix is less than one, then the gradient will be negative, meaning that we increase $\lambda_{row/col,i}$. If a row or column j of our doubly stochastic matrix is larger than one, then the gradient will be positive, meaning that we decrease $\lambda_{row/col,i}$ indefinitely. Only when a row our column i of the doubly stochastic matrix sums exactly to one, then the gradient will be zero.

This suggests an iterative approach. While the gradient of both are non-zero

- Use gradient descent to find $\tilde{q}(\lambda)$.
- Use one gradient descent step to update λ.

In the end, we have reached a local optimum that also satisfies the constraints. A large advantage of using this lagrangian multiplier method is that we have an unconstrained optimization problem now.

5.2.5 NOTEARS for VAR(1) models

We can use the NOTEARS approach also for VAR(1) models. For this, we need to make a couple of modifications.

Changes to the loss function $\ell(W;\mathbf{X})$. We change the loss from

$$\ell(W;\mathbf{X}) = \|\mathbf{X} - \mathbf{X}W\|_F^2$$

to

$$\ell(W;\mathbf{X}) = \frac{1}{2(n-1)}\|X_{[1:T]} - X_{[0:T-1]}W\|_F^2.$$

Consequently, the gradient then becomes

$$\nabla\ell(W;\mathbf{X}) = -\frac{1}{n-1}X_{[0:T-1]}\|X_{[1:T]} - X_{[0:T-1]}W\|_F.$$

Changes to the DAGness $h(W)$. The function $h(W)$ from NOTEARS was designed such that

$$h(W) = 0 \iff G(W) \text{ is a DAG.}$$

However, for our VAR(1) models, we do allow for self-loops. Therefore, we need to adjust the function $h(W)$ accordingly. Originally, the function was

$$h(W) = e^{W \circ W},$$

where $\circ$ represents the Hadamard-Product, or the element-wise multiplication of two matrices of equal dimension. The required modification is quite simple. We simply set all diagonal entries of W to zero. In other words, we propose the following function for VAR(1) models:

$$h'(W) = e^{\tilde{W} \circ \tilde{W}},$$

where the entries of $\tilde{W}$ are

$$\tilde{w}_{ij} = \begin{cases} w_{ij} & \text{if } i \neq j \\ 0 & \text{if } i = j. \end{cases}$$

Changes to the set-up. Apart from these two fundamental changes, some other minor changes needed to be done to be done to the NOTEARS repository to ensure the method also works for VAR(1) models. Firstly, we have added a method that, given a weighted adjacency matrix W, simulates data according to the VAR(1) model. Secondly, we have added the possibility for self-loops when generating the weighted adjacency matrix W. Lastly, we adjusted the bounds of the optimization procedure such that diagonal entries were not constrained to zero.

Furthermore, the elements in W were in the range of $[-2, -0.5] \cup [0.5, 2.0]$ for the original NOTEARS paper, where they assumed a SEM model. This is perfectly fine in their setting. In the VAR(1) setting, however, we must be extra careful with the diagonal entries. If they are in absolute value larger than one, we get a non-stationary series, which keeps growing. Furthermore, if one of the diagonal entries is negative, then we will see an oscillating behavior, because the sign will change with every timestep. Although this is not necessarily an issue, it is highly unlikely for any real dataset to have such an oscillating behavior. Therefore, we will keep the values on the diagonal between zero and one.

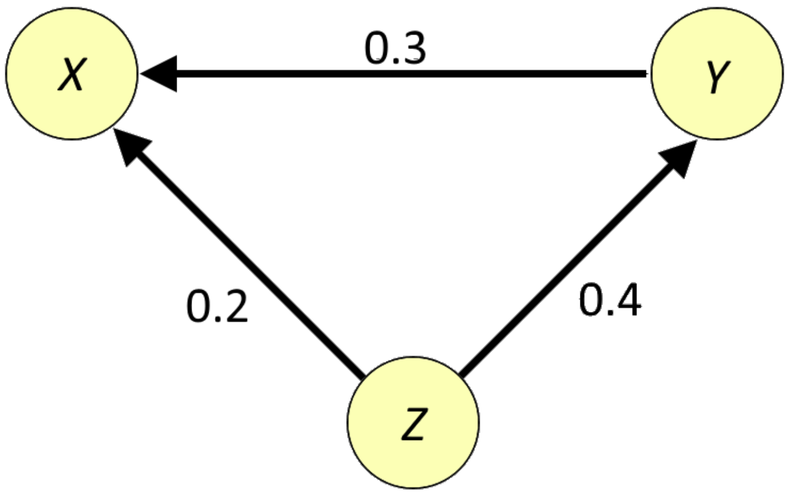


Figure 5.1: Graph of the model defined in Equation 5.11.

5.2.6 Learning a DAG by learning a permutation

We assume the model

$$\mathbf{X}_t = A\mathbf{X}_{t-1} + \epsilon$$

Now, we are looking for a permutation π, or equivalently, a permutation matrix P, such that PA is strictly lower triangular. Here, A denotes the weighted adjacency matrix (WAM).

$$G(A) \text{ is a DAG } \iff \exists \text{ a permutation matrix P s.t. } PAP^T \text{ is lower triangular.}$$

To find this permutation matrix, we will relax the constraints on P. Rather than requiring P to be a permutation matrix, we will require P to be *doubly stochastic*. This means that every row and every column of P must sum to one. In mathematical notation,

$$\sum_{i=1}^{p} P_{ij} = \sum_{j=1}^{p} P_{ij} = 1, \ \forall\ i = 1, \cdots, p, j = 1, \cdots, p.$$

To give a more concrete example, consider the model defined in Equation 5.11, consisting of three variables X, Y, and Z.

$$\mathbf{X}_t = \begin{pmatrix} X_t \\ Y_t \\ Z_t \end{pmatrix} = \begin{pmatrix} 0.4 & 0.3 & 0.2 \\ 0 & 0.5 & 0.4 \\ 0.9 & 0.0 & 0.0 \end{pmatrix} \begin{pmatrix} X_{t-1} \\ Y_{t-1} \\ Z_{t-1} \end{pmatrix} + \begin{pmatrix} \epsilon_t & 0 & 0 \\ 0 & \epsilon'_t & 0 \\ 0 & 0 & \epsilon''_t \end{pmatrix}, \tag{5.11}$$

Writing out the matrix multiplications yields the model

$$\begin{aligned} X_t &= 0.4X_{t-1} + 0.3Y_{t-1} + 0.2Z_{t-1} + \epsilon_t, \\ Y_t &= 0.5Y_{t-1} + 0.4Z_{t-1} + \epsilon'_t, \\ Z_t &= 0.9Z_{t-1} + \epsilon''_t. \end{aligned}$$

When using arrows to express dependencies in Equation 5.11, will result the graph depicted in Figure 5.1. Self-loops denoting the dependence of the variable on its own past were omitted, and the edge labels denote the weight of each edge.

Clearly, we see that (X, Y, Z) is not a topological ordering, as X_t depends on both Y_{t-1} and Z_{t-1}. However, we see that (Z, Y, X) is a valid topological ordering, as each variable only depends on its predecessors. Therefore, we are interested in learning this topological ordering, or equivalently, learning a permutation matrix P such that PAP^T is lower triangular. Ideally, we would like to retrieve the following P and A:

$$P = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \qquad A = \begin{pmatrix} 0.9 & 0 & 0 \\ 0.4 & 0.5 & 0 \\ 0.2 & 0.3 & 0.4 \end{pmatrix}.$$

Example 5.2.1. Let us consider the model given in Equation 5.12:

$$X_t = aX_{t-1} + \epsilon_t, \qquad Y_t = X_{t-1} + \epsilon'_t, \tag{5.12}$$

where $a \in [0, 1)$, and ϵ_t and ϵ'_t are both independently and identically distributed standard normal variables for all values of $t = 1, ..., T$. This model can be interpreted as X_t being some noisy hidden state variable, and Y_t being a noisy observation of the hidden state X at time $t - 1$.

Clearly, X_{t-1} is more useful for predicting Y_t than Y_{t-1} is for predicting X_t. If we know X_{t-1}, then we know Y_t up to some noise ϵ'_t. However, if we know Y_{t-1}, then we know X_{t-1} up to some noise $-\epsilon'_t$, and more importantly, we only know X_t up to this noisy estimate of X_{t-1} multiplied by a, plus an additional noise ϵ_t. Therefore, when we want to decide on the directionality of the predictive effect (so $X \to Y$ or $X \leftarrow Y$), we want our method to choose the direction $X \to Y$.

Minimization method. For this simple example with two one-dimensional variables, we can work out our model by hand. For this, we define our minimization problem as follows:

$$\arg \min_{P \subseteq \mathcal{P}, A \in \mathbb{R}^{2\times 2}} \sum_{t=2}^{T} ||P\mathbf{X}_t - AP\mathbf{X}_{t-1}||_2^2. \tag{5.13}$$

Here, $\mathcal{P}$ is the set of all doubly stochastic 2×2 matrices, and A is a 2×2 upper triangular matrix. Interestingly, a two-dimensional doubly stochastic matrix P can be uniquely defined by only one entry. As P must be doubly stochastic, both diagonal entries must be equal, which we define to be p. As both rows and columns must both sum to 1, we know that both off-diagonal entries must be equal to $1 - p$. This value $p \in [0, 1]$ denotes how likely the permutation will be. If p is close to zero, then the permutation (Y, X) is more likely, hence $X \to Y$. If p is close to one, then the permutation (X, Y) is more likely, hence $X \leftarrow Y$. Writing out this two-dimensional scenario yields the following doubly stochastic matrix P and upper triangular matrix A:

$$P = \begin{pmatrix} p & 1-p \\ 1-p & p \end{pmatrix}, \qquad A = \begin{pmatrix} a_{11} & a_{12} \\ 0 & a_{22} \end{pmatrix}.$$

Then, the minimization problem of Equation 5.13 becomes

$$\arg\min_{p\in[0,1], a_{11}, a_{12}, a_{22} \in \mathbb{R}} \sum_{t=2}^{T} \left\| \begin{pmatrix} p & 1-p \\ 1-p & p \end{pmatrix} \begin{pmatrix} X_t \\ Y_t \end{pmatrix} - \begin{pmatrix} a_{11} & a_{12} \\ 0 & a_{22} \end{pmatrix} \begin{pmatrix} p & 1-p \\ 1-p & p \end{pmatrix} \begin{pmatrix} X_{t-1} \\ Y_{t-1} \end{pmatrix} \right\|_2^2. \tag{5.14}$$

To gain a deeper understanding of Equation 5.14, let us consider the boundary values that p can attain. When $p = 0$, this yields the model

$$X_t = a_{22}X_{t-1}, \qquad Y_t = a_{11}Y_{t-1} + a_{12}X_{t-1}. \tag{5.15}$$

When $p = 1$, this yields the model

$$X_t = a_{11}X_{t-1} + a_{12}Y_{t-1}, \qquad Y_t = a_{22}Y_{t-1}. \tag{5.16}$$

If $0 < p < 1$, we will get a mixture of these two equations:

$$\begin{aligned} pX_t + (1-p)Y_t &= a_{11}\left(pX_{t-1} + (1-p)Y_{t-1}\right) + a_{12}\left((1-p)X_{t-1} + pY_{t-1}\right), \\ pY_t + (1-p)X_t &= a_{22}\left((1-p)X_{t-1} + pY_{t-1}\right). \end{aligned} \tag{5.17}$$

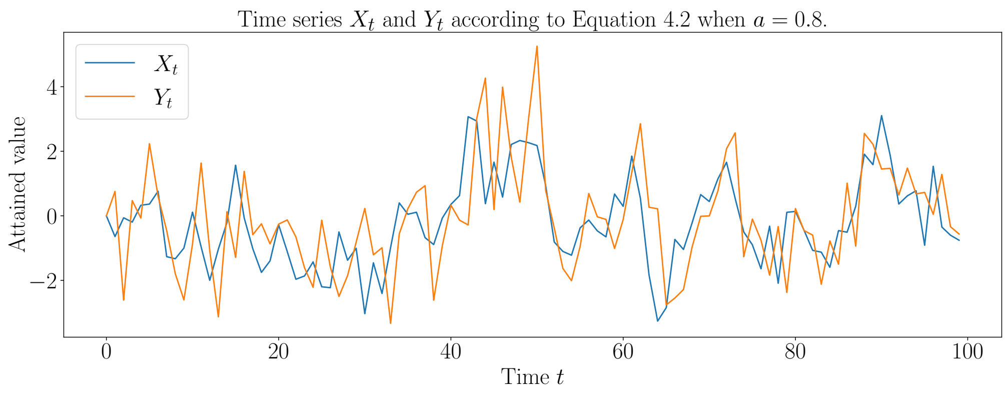


Figure 5.2: Vizualization of time series X_t and Y_t according to Equation 5.12 with $a = 0.8$.

Equation 5.12 for $a = 0.8$. Let us consider a concrete instance of Equation 5.12. We have generated a time series with time horizon $T = 100$ according to Equation 5.12 with $a = 0.8$. The resulting time series are plotted in Figure 5.2.
Applying our minimization technique from Equation 5.14, this yielded the following estimates:

$$\hat{p} = 0.35, \qquad \hat{A} = \begin{pmatrix} -1.06 & 1.98 \\ 0 & 0.853 \end{pmatrix}.$$

We see that the value for p is significantly smaller than 0.5, which would indicate that it is better to use X_{t-1} to predict Y_t than to use Y_{t-1} to predict X_t. Hence, our method suggests that the predictive effect $X \to Y$ is larger than the predictive effect $X \leftarrow Y$, just as we would expect. Therefore, this method produces the correct outcome.

Unfortunately, the matrix $\hat{A}$ does not resemble the original matrix A. The reason for this is that our value for p is still quite far away from either zero or one, and hence our model is a mixture of the equations as described in Equation 5.17. When we would force p to be either zero or one, for example by rounding p to the nearest integer, the minimization problem in this scenario becomes

$$\underset{a_{11},a_{12},a_{22}\in\mathbb{R}}{\arg\min} \sum_{t=2}^{T} \left\| \begin{pmatrix} Y_t \\ X_t \end{pmatrix} - \begin{pmatrix} a_{11} & a_{12} \\ 0 & a_{22} \end{pmatrix} \begin{pmatrix} Y_t \\ X_t \end{pmatrix} \right\|_2^2. \tag{5.18}$$

Solving Equation yields the following estimate of A:

$$\hat{A} = \begin{pmatrix} 0.01 & 1.01 \\ 0 & 0.80 \end{pmatrix},$$

which is very close to the actual model.

Values of p in Equation 5.12 for different values of a To see the influence of the coupling strength of a, we have tried different values for a and computed the corresponding value for p. These results are shown in Figure 5.3.

We see that as a increases, the value for p decreases. In other words, as we increase the dependence of Y_t on X_{t-1}, the value for p decreases towards zero, meaning the data leans more towards Equation 5.15 rather than Equation 5.16. Given that we generated the data according to Equation 5.15, this is as expected. However, the decrease is not as steep as we would have hoped; the values for p are indeed smaller than 0.5, but also remain larger than 0.3 for all suitable values of a.

Example 5.2.2. *Two-dimensional AR(1) model.*
Now consider the more generic two-dimensional model

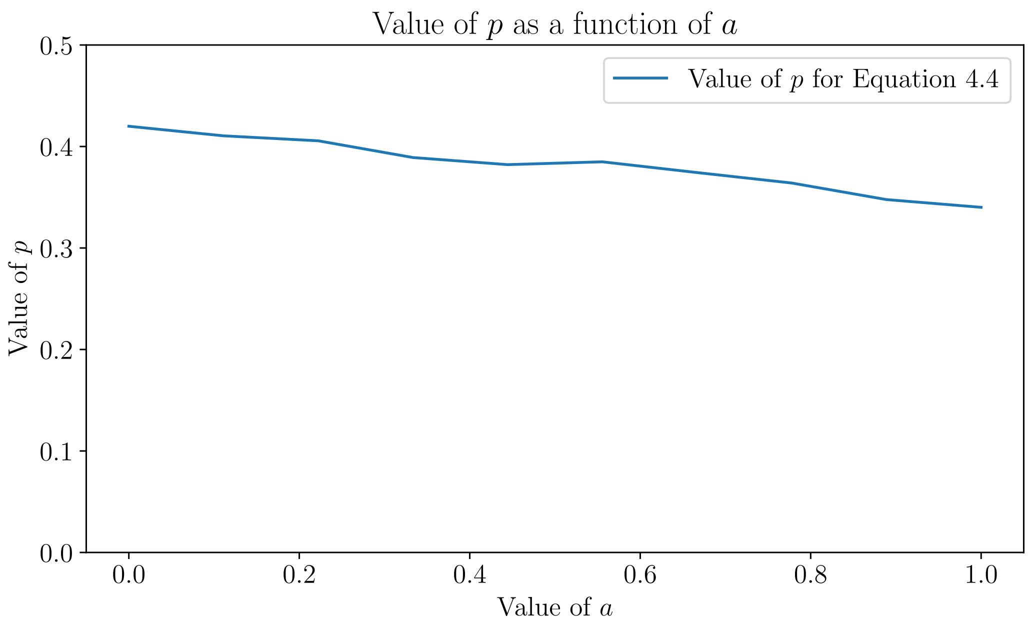


Figure 5.3: Value of p as a function of a in Equation 5.12.

$$\begin{pmatrix} X_t \\ Y_t \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} X_{t-1} \\ Y_{t-1} \end{pmatrix} + \begin{pmatrix} \epsilon_t \\ \epsilon'_t \end{pmatrix}. \tag{5.19}$$

Equation when $a_{11} = a_{22}$ and $a_{12} = a_{21}$. Let us consider the scenario where X and Y predict each other equally.

$$X_t = aX_{t-1} + bY_{t-1} + \epsilon_t,$$
$$Y_t = aX_{t-1} + bY_{t-1} + \epsilon'_t.$$

From this equation, we can clearly see that X_{t-1} predicts Y_t equally well as Y_{t-1} predicts X_t. Hence, we would expect our method to report values of p close to a half. We have created a contour plot in Figure that shows the value of p for a given pair (a, b). Note that the contour plot concerns only pairs (a, b) where $a + b < 1$, as larger values would mean that X and Y would diverge towards either positive or negative infinity.

We see that for all pairs (a, b), the value p remains close to a half. The small deviations of p are most likely caused by the randomness of ϵ_t and ϵ'_t.

Equation when $a_{12} = a_{22} = 0$. We are also interested in the scenario where X is a clear influencer of Y, so

$$X_t = a_{11}X_{t-1} + \epsilon_t$$
$$Y_t = a_{21}X_{t-1} + \epsilon'_t$$

Clearly, X_{t-1} is a useful predictor for Y_t. The question is how much the parameters a_{11} and a_{21} influence the values of p for detecting the direction of this predictive effect. Lower values of a_{21} decrease the predictive effect of X_{t-1} on Y_t, as the noise component ϵ'_t becomes more dominant. Furthermore, lower values of a_{11} result in smaller values of X_t, which also results in the noise component ϵ'_t to become more dominant.

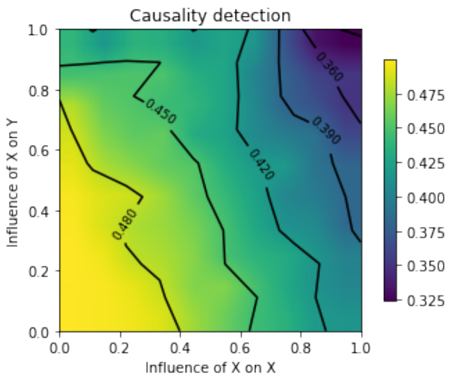


Figure 5.4: first figure

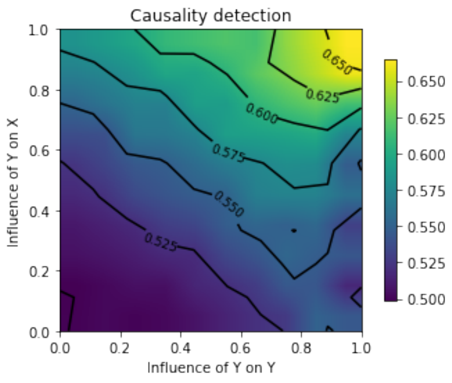


Figure 5.5: second figure

We have created a contour plot in Figure that shows the value of p for a given pair (a_{11}, a_{21}). A brighter more yellow color indicates that p is close to 0.5. A darker more blueish color indicates that p is smaller than 0.5. Figure tells us that indeed, the value of p increases as either a_{11} or a_{21} increases, indicating that the predictive effect $X \to Y$ increases. This is in line with what was expected.

To verify whether our approach is symmetric, we will also investigate where the roles of X and Y are switched around, so now $a_{11} = a_{21} = 0$. As Y_{t-1} is now a more useful predictor of X_t, we expect higher values for p. Just as for the previous example, we expect larger values for both a_{12} and a_{22} to yield larger values for p. We have created a countour plot in Figure that shows the values of p for a given pair (a_{12}, a_{22}).

In Example 1 and Example 2, we have seen that our method seems to perform well in the simple two-dimensional setting, reporting the correct direction of the predictive effect. Furthermore, when there is no predictive effect, the method reports this as well. Lastly, when the predictive effect is equal in both directions, the method does not pick sides. The question remains whether this method will also work in higher dimensions.

Example 5.2.3. *Three dimensions.* Now, consider the three dimensional setting from Equation 5.11. Just as in Example 4.1.1, we expect our method to report $X \leftarrow Y \leftarrow Z$. The main difference between the two and the three dimensional case is that we now need more parameters for our doubly stochastic matrix P. As it turns out, we require $(n-1)^2$ parameters for an $n \times n$ doubly stochastic matrix. If we take all entries except the bottom row and the right-most column as parameters, $\{p_{ij}\}_{i,j=1,\dots,n-1}$, we can deduce all other values. First, we can deduce the right-most entry for each of the top $n-1$ rows, as the entries in each row must sum to one, so $p_{in} = 1 - \sum_{j=1}^{n-1} p_{ij}$. Similarly, we can deduce the bottom entry for each of the left-most $n-1$ columns by $p_{nj} = 1 - \sum_{i=1}^{n-1} p_{ij}$. Lastly, we can deduce the bottom-right right entry by either using the right-most column or the bottom row by $p_{nn} = 1 - \sum_{i=1}^{n-1} p_{in} = 1 - \sum_{j=1}^{n-1} p_{nj}$. Hence, we now require 4 variables, which we denote by $\{p_{ij}\}_{i,j=1,2}$ to uniquely define the three-dimensional doubly stochastic matrix P.

Generating data according to this model and applying our method yielded the following estimates for $\hat{P}, \hat{A}$:

Closest permutation matrix by Hungarian algorithm.

5.3 Combinatorial Approaches

In this section, we will discuss approximate methods that are combinatorial in nature. The difficulty that arises when using this type of method is that the combinatorial search space of DAGs is super exponential. Nevertheless, our approaches here focus on finding a permutation matrix P and a lower triangular matrix A. Given a permutation matrix P, finding a suitable lower triangular matrix is quite simple, for example the closed form least-squares solution. Nevertheless, the total number of permutation matrices on p variables is $p!$, which also grows exponentially with respect to p. This section considers some of these combinatorial methods of different complexities.

5.3.1 Exhaustive Search

A simple and naive method is to simply try all potentially optimal weighted adjacency matrices. Unfortunately, it is not straightforward to find this set of potentially optimal matrices. Luckily, the decomposition first described in Chapter 2 is useful here. We can decompose our weighted adjacency matrix W into an upper triangular matrix A and a permutation matrix P, i.e.,

$$W = P^T AP.$$

To find the optimal weighted adjacency matrix W, we need to iterate over all such sensible pairs A and P. We can now utilize a principled approach using this decomposition, which we call "DAG-OLS".

DAG-OLS Interestingly, once we are given a permutation matrix P, there is a closed-form solution to find the optimal upper triangular matrix A that adheres to this permutation P. This is the *ordinary least squares* solution, where we regress a variable on only the variables that precede it in the permutation, as well as the variable itself. More concretely, for the variable that occurs first in the permutation, we regress it only on itself. For the second variable that occurs in the permutation, we regress it only on itself and all the preceding variables, which in this case is only the first variable in the permutation. More generally, for the ith variable in the permutation, we regress it on itself, as well as the $i - 1$ variables that precede it in the permutation. This procedure yields the matrix A that minimizes the Mean Squared Error, while still adhering to the aforementioned permutation matrix P. `DAG-OLS` is described in Algorithm 4.1.

Algorithm 4.1 DAG-OLS

Input: Data matrix X, Permutation matrix P.
Output: Upper triangular matrix A that minimizes the Mean Squared Error for X, respecting permutation P.

```
 1: $X_P \leftarrow XP^T$                                  ▷ Swap columnsof $X$
 2: $A \leftarrow \mathbf{O}_{p\times p}$                  ▷ Initialize $A$ as $p \times p$ zero matrix
 3:
 4: $Y \leftarrow X_P[2:T]$                                ▷ Get endogeneous variable $Y$
 5: $X_{pred} \leftarrow X_P[1:T-1]$                       ▷ Get exogeneous variable $X$
 6:
 7: for $i = 1$ until $p$ do
 8:     $X_i \leftarrow X_{pred}[1:i]$                     ▷ Data of first $i$ variables in $P$
 9:     $Y_i \leftarrow Y[i]$                              ▷ Data of $i$th variable in $P$
10:     $A[1:i][i] = \left(X_i\ X_i^T\right)^{-1} X_i^T Y_i$   ▷ Perform OLS for variable $i$
11: end for
12:
13: $W \leftarrow P^T AP$                                  ▷ Transpose rows and columns of $A$
14: return $W$
```

A step-by-step three dimensional example showcasing the inner workings of DAG-OLS is given in Example 5.1.

Example 5.1 DAG-OLS with three variables.

Let us give an example of how DAG-OLS works. Suppose that we have three variables, and we are given an ordering $\pi = (3, 1, 2)$, corresponding to the permutation matrix

$$P = (e_3^T, e_1^T, e_2^T) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

Using the DAG-OLS algorithm, this means that for the third variable, we can only use the variable itself. For the first variable, we use the variable itself and all preceding variables, so the first and third variable. Finally, for the last variable, we can use all three variables.

Now, we can find the matrix A that minimizes the Mean Squared Error using while still adhering to the permutation matrix P. We can do this by using ordinary least squares, where we regress the ith variable on only the preceding variables and the ith variable itself. Let Y_i be the variable that we regress on at the ith iteration, and let X_i represent the i variables used when regressing on Y_i. The closed-form solution for the coefficients in the ith column then is

$$A[i][i:p] = \left(X_i X_i^T\right)^{-1} X_i^T Y_i,$$

which also occurs on line 10 of algorithm 4.1. Returning to our example, let X represents the first $T-1$ samples that we use to predict the last $T-1$ samples, which are represented by Y. Let the subscripts of X and Y denote the subset of variables used in the regression. This means that the first column of A we have that

$$A[1:3][1] = \left(X_3 X_3^T\right)^{-1} X_3^T Y_3.$$

For the second column, we already know that the first entry must be equal to zero to ensure that A remains lower triangular. Hence, we fill A starting from the diagonal entry. Therefore, we have for the second column of A that

$$A[2:3][2] = \left(X_{3,1} X_{3,1}^T\right)^{-1} X_{3,1}^T Y_1.$$

When we estimate the coefficients of the final column, we only have one entry, for which we use all the variables X_1 until X_3. Do note, however, that the variables are swapped around in $X_{3,1,2}$, to ensure that we adhere to the permutation of our data matrix X, conform the first line of algorithm 4.1. As last entry, we have

$$A[3][3:3] = A[3][3] = \left(X_{3,1,2} X_{3,1,2}^T\right)^{-1} X_{3,1,2}^T Y_2.$$

As a final procedure, we permute the rows and columns of A back from the permutation $\pi = (3, 1, 2)$ to the numerical ordering $(1, 2, 3)$, which is done by

$$W = P^T A P.$$

This matrix W that has been returned is the matrix that minimized the Mean Squared Error with respect to our data X, while still respecting the ordering imposed by our permutation matrix P.

Exhaustive Search Now, we have found a way to find the optimal A given a permutation matrix P. What remains is to perform an exhaustive search over all possible permutation matrices $P_{perm} \in \mathcal{P}$. An overview of the algorithm is given in Algorithm 4.2.

Algorithm 4.2 Exhaustive-Search

Input: Data matrix X.
Output: WAM W that minimizes the Mean Squared Error.

```
W_best ← $I$
MSE_best ← $\infty$

for every permutation matrix $P$ do
    $A \leftarrow$ DAG-OLS($P$)
    $W \leftarrow P^T A P$
    if MSE($W$) < MSE_best then
        MSE_best ← MSE($W$)
        W_best ← $W$
    end if
end for

return W_best
```

Unfortunately, When we have p variables, there is a total of $p!$ possible permutations, which is not tractable when we have a large number of variables p. The exhaustive algorithm has been implemented in Python and unfortunately does not support more than ten variables. In such a scenario, a total of 10!, approximately 3.6 million lower triangular matrices A need to be estimated, which implies that we regress a total of 36 million times. Nevertheless, investigating this problem in relatively small dimensions provides an interesting starting point which can provide insightful discoveries. When applying the algorithm to eight variables and one thousand samples per variable, the algorithm takes approximately one minute to return the optimal matrix W.

A large upside of the exhaustive search method is that the returned method is guaranteed to be *optimal*. To see this, recall that we defined "optimal" to be the weighted adjacency matrix W that minimizes the Mean Squared Error. Interestingly, the DAG-OLS algorithm guarantees to return the lower triangular matrix A that is the is the exact minimizer of the Mean Squared Error with respect to a given permutation matrix P. As we simply try all permutation matrices P, the exhaustive approach is guaranteed to return the optimal weighted adjacency matrix W. This showcases the trade-off between the running time of our algorithm and the quality of its output. The algorithm outputs the optimal matrix, at the cost of having an exponential running time of $\mathcal{O}(p!)$.

Number of suitable permutations An interesting remark is that sometimes we do not need to do an exhaustive search of all permutation matrices to find the optimal solution, especially when the true matrix W is sparse. In fact, any permutation that adheres to the topological ordering of the graph $G(W)$ would yield the same optimal solution for a large enough sample size. If for example, the fourth and the fifth variable do not depend on each other, so $W_{4,5} = W_{5,4} = 0$, then it does not matter which variable precedes the other in the permutation. Hence, there could be multiple permutations matrices P such that $P^T AP$ is upper triangular.

Example 5.2 Total number of possible orderings

Let us give an example of what we mean when we say that multiple permutation matrices will yield the optimal solution. Suppose that our data is generated according to a VAR(1) model with five variables and coefficient matrix

$$W = \begin{pmatrix} 0.5 & 0.5 & 0.0 & 0.0 & 0.5 \\ 0.0 & 0.5 & 0.0 & 0.5 & 0.0 \\ 0.0 & 0.0 & 0.5 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.5 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.5 \end{pmatrix}.$$

For easy of notation, our matrix W is already an upper triangular matrix. However, we could have simply permute this using any permutation matrix P, although it would make it more difficult to see which orderings are also valid. Furthermore, the value of the coefficients is not important here, so all coefficients simply have a value of 0.5.

Now, it is clear that the ordering $(1, 2, 3, 4, 5)$ is a permutation such that we can estimate all non-zero coefficients of W, as

$$W = I^T A I,$$

for some upper triangular matrix A. Hence, using DAG-OLS with permutation I will unveil all true coefficients, assuming our sample size is large enough.

However, this is not the only permutation we can think of. First of all, our third variable only depends on itself, so this variable can be at any index in the permutation and our matrix W will still be upper triangular. This already increases the number of appropriate orderings from just 1 to 5. Furthermore, since the fourth and fifth variable do not depend on each other, we can interchange them in which way we like. Lastly, since the fifth variable only depends on the first variable, we only need to ensure that the first variable precedes the fifth variable. In total, there are a total of 20 permutation P such that $P^T W P$ remains upper triangular, thereby implying that DAG-OLS can estimate all true coefficients.

This means that out of the 5! permutations, 20 permutations are suitable for estimating all true coefficients, so we often do not need to check *all* possible permutations.

In Example 5.2, we have seen that there often are quite some possible permutation matrices P to properly estimate our matrix W. Especially when the matrix W is sparse, there are quite some permutation matrices possible. The question that arises now is the following: "Given a matrix W, how many different permutations of its rows and columns are there that yield an upper triangular matrix?" In other words, how many permutations are there such that DAG-OLS can estimate all non-zero coefficients of W? Unfortunately, this is a difficult question to answer. In fact, this problem is #P-Complete [4], meaning that this problem is even harder than an NP-Complete problem Therefore, the only statement we can make that for a sparse W, there are most likely quite some valid orderings of the variables. How many there are is, unfortunately, often too difficult to compute. Nevertheless, a code snippet has been provided that naively computes the number of suitable permutations has been provided in Appendix A.1. It takes approximately seven minutes to count the number of suitable permutations for ten variables.

As a sidemark, note that a sparse matrix does not always imply that there exist many possible permutations. Consider the matrix with non-zero coefficients on the diagonal above the main diagonal, which is also called the *superdiagonal*:

$$W = \begin{pmatrix} 0.0 & 0.5 & 0.0 & \cdots & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.5 & \cdots & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & \cdots & 0.0 & 0.0 & 0.0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0.0 & 0.0 & 0.0 & \cdots & 0.0 & 0.5 & 0.0 \\ 0.0 & 0.0 & 0.0 & \cdots & 0.0 & 0.0 & 0.5 \\ 0.0 & 0.0 & 0.0 & \cdots & 0.0 & 0.0 & 0.0 \end{pmatrix}.$$

As each variable depends on only the preceding variable, we cannot have any ordering other than $P = I$. Therefore, the number of suitable permutations is equal to 1, although we have a sparse matrix with only $p - 1$ non-zero coefficients.

Example 5.3 Applying the exhaustive method on three variables

Consider the three-dimensional data shown in Figure 5.6. This data has been generated using the formula

$$X_{t,\cdot} = X_{t-1,\cdot}W + E_t, \tag{5.20}$$

where

$$W = \begin{pmatrix} 0.8 & 0.0 & 0.0 \\ 0.5 & 0.8 & -0.5 \\ 0.0 & 0.0 & 0.8 \end{pmatrix}, \qquad E \sim \mathcal{N}(\mathbf{0}, I_3).$$

We pre-define $X_{0,\cdot} = \mathbf{0}$, so that $X_{1,\cdot} = E_1$, and $X_{t,\cdot}$ follows from Equation 5.20. We simulate for a total of $T = 100$ timesteps.

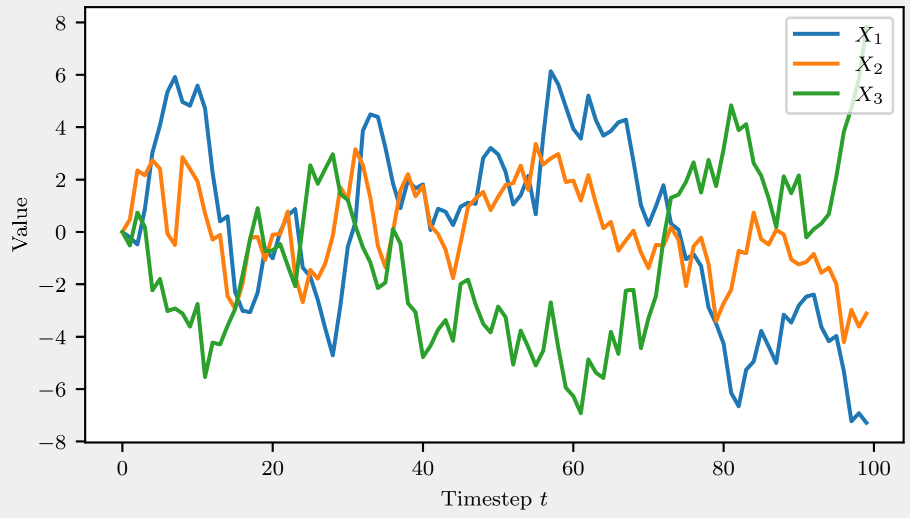


Figure 5.6: Vizualisation of the three variables X_1, X_2, X_2 of Example 5.3.

Now, our exhaustive search as described in Algorithm 4.2 will simply iterate over all possible permutation matrices P, of which there are a total of $3! = 6$. For each permutation matrix, we calculate the ordinary least squares coefficient matrix A using only coefficients in the upper triangular part of $P^T AP$ using `DAG-OLS`(X, P) described in Algorithm 4.1. Let us first consider where we use the identity matrix as our permutation $P_1 = I$, and hence, we can only estimate coefficients from the upper triangular part of W. Using `DAG-OLS`, we get that

$$W_{P_1} = \begin{pmatrix} 0.96 & 0.01 & -0.08 \\ 0.0 & 0.80 & -0.42 \\ 0.0 & 0.0 & 0.77 \end{pmatrix},$$

with an accompanying Mean Squared Error of 3.421.

Now, let us consider a permutation P such that `DAG-OLS` can estimate all true coefficients of W. Two permutations satisfy this condition, which are

$$P_2 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad P_3 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

Applying `DAG-OLS` with these two permutation matrices P_2 and P_3 yield the respective coefficient matrices

$$W_{P_2} = \begin{pmatrix} 0.79 & 0 & -0.08 \\ 0.55 & 0.81 & -0.42 \\ 0 & 0 & 0.77 \end{pmatrix}, \qquad W_{P_3} = \begin{pmatrix} 0.77 & 0 & 0 \\ 0.55 & 0.81 & -0.48 \\ -0.02 & 0 & 0.83 \end{pmatrix},$$

with accompanying Mean Squared Errors of 2.906 and 2.930 respectively. As we can see, both estimate all true coefficients, but one achieves a slightly lower Mean Squared Error. As our data is corrupted with noise, non-true coefficients are also estimated with small coefficients that overfit on the noise in the data. Apparently, overfitting on the noise with coefficient $w_{3,1}$ yields better results than with coefficient $w_{1,3}$.

Table 5.1: Table Showing the Mean Squared Errors of all six possible permutations for Example 5.3. A lower Mean Squared Error implied a better fit. Both permutation $P_2 = (2, 1, 3)$ and $P_3 = (2, 3, 1)$ achieve a low Mean Squared Error, as they estimate all true coefficients of W. P_2 overfits slightly better on the noise, resulting in a slightly lower Mean Squared Error. All other permutations fail to estimate at least one true coefficient of W, resulting in a larger Mean Squared Error and hence, a poorer fit.

Permutation	(1, 2, 3)	(1, 3, 2)	(2, 1, 3)	(2, 3, 1)	(3, 1, 2)	(3, 2, 1)
Mean Squared Error	3.421	3.724	2.906	2.930	3.927	3.413

As a final remark, the results of all six permutations are shown in Table 5.1, where we indeed see that the lowest Mean Squared error is achieved by P_2. The code used to generate this example has been provided as a Jupyter Notebook in Appendix.

Final Remarks We see that, although the problem we are tackling is NP-hard, the problem becomes simple when a suitable permutation is provided. However, finding this permutation is quite difficult. Using an exhaustive search, we can iterate over all permutations and we are guaranteed to find the optimal W. Iterating over all possible permutations of our variables unfortunately implies that the running time is exponential with respect to the number of variables p, namely $\mathcal{O}(p!)$.

5.3.2 Random Walk

In Subsection 5.3.1, we have seen that we can find our optimal matrix W by trying all possible permutations of rows and columns of W. Unfortunately, there are $p!$ of those permutations, where p is the number of variables or equivalently, the number of rows or columns in W. Therefore, we cannot expect to find the optimal permutation within a reasonable amount of time. Nevertheless, we can try to find a reasonably good permutation without checking all the possible permutation matrices. For this, we can do a *random walk* through the space of permutation matrices $\mathcal{P}_{perm}$. For each permutation, we apply `DAG-OLS`(X, P) to see whether this permutation matrix P is a good fit for our data X. We fix the number of permutations we visit to a certain number N or alternatively, we set the maximum time that can elapse during our random walk to a fixed time of T_{max}.

There are two decisions to be made with respect to our random walk:

1. The method of deciding the next step. In a random walk, the next step, or in our setting the next permutation matrix, is often chosen uniformly at random from a set of candidates. There are two main choices to define the next set of candidates.

   First of all, we can just simply pick one at random from the $p!$ possible candidate permutation matrices. Note that this also includes our current state, from which we do not gain any information by revisiting this permutation. Therefore, it may be wise to exclude already visited permutation matrices from our set of matrices. However, when p is large, the probability of visiting the exact same permutation matrix is quite small, and remembering all visited permutation matrices may take quite some storage without improving the algorithm significantly. So, our decision rule would be

$$P_{next} = \mathcal{P}^{(i)}_{perm} \text{ with probability } \frac{1}{p!}, \tag{5.21}$$

where $\mathcal{P}_{perm}$ is the set of all possible permutation matrices on p variables.

Secondly, we can define the set of candidates as the set of permutation matrices that are "closest" to our current permutation matrix P. We define the set of "closest" permutation matrix as the set of permutation matrices that can be reached by flipping the order of just two variables. In mathematical notation, we have that

$$\mathcal{P}_{closest(P)} = \{P' \mid \text{swap row } i \text{ and } j \text{ of } P,\ i = 2, \dots p,\ j = 1, \dots, i-1.\}. \tag{5.22}$$

In total, there are $\binom{p}{2}$ of such permutation matrices P' for any permutation matrix P. We pick one permutation matrix P' uniformly at random from this set (so with probability $1/\binom{n}{2}$). Our decision rule would then be

$$P_{next}(P) = \mathcal{P}^{(i)}_{closest(P)} \text{ with probability } \frac{1}{\binom{n}{2}}. \tag{5.23}$$

2. The starting permutation of the random walk. The random walk must start at some permutation matrix P. For the second case, where we only move to one of the "closest" permutation matrices P', the initial starting point P_0 greatly determines which permutation matrices we will visit. For example, suppose that we start at $P_0 = I_p$, how many steps must we take to visit the exact opposite permutation, so the backwards identity matrix

$$J_p = \begin{pmatrix} 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & 1 & 0 \\ \vdots & \vdots & \iddots & \vdots & \vdots \\ 0 & 1 & \cdots & 0 & 0 \\ 1 & 0 & \cdots & 0 & 0 \end{pmatrix}?$$

   This is a difficult questions, but for now, it seems to be of the order $\mathcal{O}(p!)$. Therefore, starting with a permutation "far" from a good permutation can result in a long waiting time before we find a suitable permutation.

   Note that for our first choice, the initial permutation matrix does not matter at all, as all $p!$ permutation matrices are equally likely to be next permutation matrix.

Remark: Very interesting question, given the set of integers $[[p]] = \{1, 2, \dots, p\}$, how often do we need to swap to number uniformly at random until we have reached $\{p, p-1, \dots, 1\}$?

Both versions of the random walk are given in Algorithm 4.3. Note that they differ in the way they sample the next permutation matrix P_n. For the completely random walk, we use Equation 5.21 to determine the next permutation P_n. For the random walk where the next step to the permutation matrices that differ by only one transposition of two rows, we use Equations 5.22 and 5.23.

Algorithm 4.3 Random Walk

Input: Data matrix X, Initial permutation P_0, maximum number of steps N.
Output: WAM W.

```
1: W_best ← $P_0$
2: MSE_best ← MSE($P_0$)
3:
4: for $n = 1$ until $N$ do
```

```
 5:     $P_n \leftarrow$ P_next($P_{n-1}$)
 6:     $A \leftarrow$ DAG-OLS($P_n$)
 7:     $W \leftarrow P_n^T A P_n$
 8:     if MSE($W$) $<$ MSE_best then
 9:         MSE_best $\leftarrow$ MSE($W$)
10:         W_best $\leftarrow W$
11:     end if
12: end for
13:
14: return W_best
```

Determining the initial state of the random walk. As mentioned before, the initial permutation matrix of the random walk, P_0, can greatly affect the quality of the outcome. When the next state of the random walk is limited to permutation matrices that are one transposition away from its current state, it may take a long time to reach permutation matrices that differ quite significantly, for example the identity matrix and the backwards identity matrix. Therefore, it is important to have a method to determine a suitable initial matrix P_0.

An effective method is to first simply do ordinary least squares on X, which yields a matrix A_{OLS}. However, as this matrix does not correspond to a directed acyclic graph, this is not a suitable way to determine our starting point yet. We need a method to find a matrix W that is close to A_{OLS}, yet corresponds to a directed acyclic graph. From hereon, we can determine an ordering P_0 that corresponds to W, which will be a suitable starting point.

Now, we can iteratively select the edge from the set of violating edges that results in the least harm done to our mean squared error. The set of violating edges are all the edges that are contained in at least one cycle of length greater than one. The length of the cycle must be greater than one, as self-loops, which are cycles of length 1, are allowed in our model. We can use Johnson's algorithm, coined by Johnson in [], to efficiently find all cycles of length greater than one. Johnsons algorithm is among the most efficient algorithms to find all simple cycles, and has a useful implementation in NetworkX for Python.

After we have found all violating edges, we will greedily remove the edge that is deemed the least important, in the sense that removing this edge yields the smallest increase in Mean Squared Error.

We can iteratively proceed removing the least important edge until the remaining matrix W constitutes a directed acyclic graph. We can use this matrix as our starting point.

5.3.3 Using Markov Chain Monte Carlo

As we have seen in Section, relaxing the search space from the set of permutation matrices to the set of doubly stochastic matrices created numerous issues. Although the search space is now continuous rather than combinatorial, the presence of singular or close to singular doubly stochastic matrices makes it difficult to retrieve a local optimum (A, P) such that P is "close" to a permutation matrix. This section takes one step back and tries a novel approach to find a suitable permutation matrix P.

The approach that we will investigate in this section is a so-called *Markov Chain Monte Carlo* (MCMC) method, inspired by [5].

$$q_{P,P'} = \Pr\left(s_{i+1} = P' \mid s_i = P\right) = \begin{cases} 0 & \text{if } P' \text{ is not within one move from } P \\ \frac{1}{n_P} & \text{otherwise} \end{cases} \tag{5.24}$$

Here, we define "one move" as the interchanging of two variables X_i and X_j. This is done by interchanging the ith row and the jth row or equivalently, interchanging the ith row and the jth column.

Given a permutation matrix on n variables, there are a total of $\binom{n}{2}$ possible moves. Hence, the possible number of valid moves does not depend on the permutation matrix P.

Let us now define the probability of acceptance $\alpha_{P,P'}$ as

$$\alpha_{P,P'} = \begin{cases} \min\left\{\frac{\mathcal{L}(\mathbf{X}|P')\cdot q_{P',P}}{\mathcal{L}(\mathbf{X}|P)\cdot q_{P,P'}}, 1\right\} & \text{if } \mathcal{L}(\mathbf{X} \mid P)\cdot q_{P,P'} > 0 \\ 1 & \text{otherwise} \end{cases} \tag{5.25}$$

The number of permutation matrices P' that are within one move from P is equal to the total amount of possible variables that we can swap. For any permutation matrix P, n_P is equal to the number of possible pairs given n variables, which is

$$n_P = \binom{n}{2} = \frac{n(n+1)}{2} \quad \forall P \in \mathcal{P}.$$

Now, we have that the likelihood of our data $\mathbf{X}$ given our lower triangular matrix A and our permutation matrix P is

$$\mathcal{L}(\mathbf{X}|A,P) = \frac{1}{2(T-1)}\left\|\mathbf{X}_{[1:T]} - \mathbf{X}_{[0:T-1]}P^T A P\right\|_F^2.$$

However, for a given permutation matrix P, we do not know A. Luckily, the likelihood is only quadratic with respect to A, so $\mathcal{L}(\mathbf{X}|A,P)$ can be easily be optimized with respect to A via for example gradient descent. The gradient of $\mathcal{L}(\mathbf{X}|A,P)$ with respect to A is

$$\nabla_A \mathcal{L}(\mathbf{X}|A,P) = -\frac{1}{(T-1)}P\mathbf{X}_{[0:T-1]}^T\left\|\mathbf{X}_{[1:T]} - \mathbf{X}_{[0:T-1]}P^T A P\right\|_F P^T.$$

Let

$$\mathcal{L}(\mathbf{X}|P) = \arg_A \min \mathcal{L}(\mathbf{X}|A,P).$$

Then, we get that the probability of acceptance $\alpha_{P,P'}$ is equal to

$$\alpha_{P,P'} = \begin{cases} \min\left\{\frac{\mathcal{L}(\mathbf{X}|P')}{\mathcal{L}(\mathbf{X}|P)}, 1\right\} & \text{if } \mathcal{L}(\mathbf{X} \mid P) > 0 \\ 1 & \text{otherwise} \end{cases} \tag{5.26}$$

Now, the transition matrix of the *new* Markov chain $\{r_{P,P'}\}$ is

$$r_{P,P'} = \Pr(s_{i+1} = P' \mid s_i = P) = \begin{cases} \alpha_{P,P'}q_{P,P'} & \text{if } P' \neq P \\ 1 - \sum_{P' \neq P}\alpha_{P,P'}q_{P,P'} & \text{if } P' = P \end{cases} \tag{5.27}$$

However, we need to find a “good” initialization P_0 from where we start sampling according yo our chain $\{r_{P,P'}\}$.

Initial state of $\{r_{P,P'}\}$. We can use the *ordinary least squares* estimate for W.

However, $\hat{W}$ need not be the WAM of a DAG. We will iteratively set the smallest (in absolute value) entry of $\hat{W}$ to zero until $\hat{W}$ is the WAM of a DAG.

From this initial state, we can already expect to be close to a good guess, especially when we have enough samples, i.e, T is sufficiently large.

5.3.4 Orthogonal Matching Pursuit

An interesting method that originates from regression techniques is *Orthogonal Matching Pursuit* (OMP) [11], also known as *Greedy Least Squares* regression [14] or *Orthogonal Least Squares.* In the machine learning literature, it is also known as *Forward Greedy Selection.*

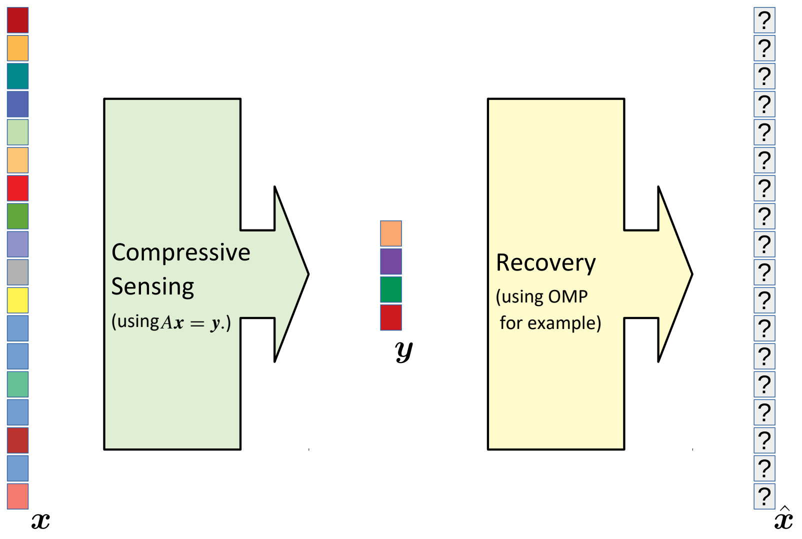


Figure 5.7: Schematic Overview of Compressive Sensing and Signal Recovery, adapted from [10].

Origin of OMP When OMP was proposed in 1993 by Mallat et. al., it was proposed as an algorithm to recover a sparse-coded signal from noisy measurements. When we talk about recovering a sparse-coded signal, we wish to recover a signal x from its compressed version y, where y has much fewer features. In such a sparse-coded signal, only a small subset of k features of y is required to recover this signal x.

Suppose that we have a large vector $x \in \mathbb{R}^n$ that is compressed using a *compression matrix* $A \in \mathbb{R}^{m \times n}$ to a smaller vector $y \in \mathbb{R}^m$. In the scenario of compressive sensing, we have

$$y = Ax.$$

For the compression to make sense, the compression matrix generally has fewer rows than columns, i.e., $m << n$, such that the compressed signal y has much dimensions than the original signal x.

Now, the original goal of Orthogonal Matching Pursuit and other signal recovery algorithms is to recover the signal x from the compressed signal y as close as possible. A visualization of the compression and recovery of a signal x is given in Figure 5.7.

Interestingly, if we wish to recover x from the compressed y and we are given the compression matrix A, then we need to solve a system of n linear equations with m unknowns. In the setting of signal recovery, n is much larger than m. So, we have much more linear equations than variables. From linear algebra, we know that there is a unique solution to a system of n independent linear equations and m variables when n is exactly equal to m. However, now that $m << n$, we have in fact infinitely many solutions. So, for a given y and A, there are infinitely many x' such that

$$Ax' = y.$$

From this, the question arises, how can we recover x from y given A?

Interestingly, although there are infinitely many solutions x, there is only one solution $\hat{x}$ which is maximally sparse [10], which means that of all x that satisfy $Ax = y$, the solution $\hat{x}$ has the fewest non-zero coefficients. To find this $\hat{x}$, we need to solve the problem

$$\hat{x} = \min_x ||x||_0 \text{ subject to } x \in \{x \mid Ax = y\}. \tag{5.28}$$

Where $||x||_0$ represents the zero-"norm" (a misnomer as it is technically not a norm), which is defined as the number of non-zero coefficients. In mathematical notation, $||x||_0 = |\{x_i \mid x_i \neq 0\}|$. However, with real life data, it is often not realistic to assume that Ax is *exactly* equal to y. Therefore, we often allow for a small tolerance ϵ in the two-norm. The problem then becomes

$$\hat{x} = \min_x ||x||_0 \text{ subject to } x \in \{x \mid ||Ax - y||_2 \leq \varepsilon\}. \tag{5.29}$$

Unfortunately, both Problem 5.28 and Problem 5.29 are NP-hard to solve, meaning that we cannot expect to find their solution within a reasonable amount of time, especially when m and n are large. Generally, this issue is cicrumvented by replacing the zero-norm with the one-norm, which is the sum of the absolute values of the elements of x. The problem then becomes

$$\hat{x} = \min_x ||x||_1 \text{ subject to } x \in \{x \mid ||Ax - y||_2 \leq \varepsilon\}. \tag{5.30}$$

Another option is to use a greedy approach to approximately solve Problem 5.29. Greedy approaches iteratively select and estimate the zero-valued coefficient x_i that results in the largest gain. This iterative process continues until some stopping criterion is met. Examples of such algorithms used for compressive sensing are Matching Pursuit [11], Iterative Hard Thresholding [3], and the method that we will be applying to our problem, Orthogonal Matching Pursuit [11]. The difference between these three methods are the selection procedure and the stopping criterion, but the general approach is these three methods is quite similar.

OMP as a Greedy Least Squares regression. Apart from the signal processing community, Orthogonal Matching Pursuit is now also widely used in machine learning. Suppose that we have a data matrix $X \in \mathbb{R}^{n \times m}$, and we want to regress these on our variable $y \in \mathbb{R}^m$ using a linear form of regression, so

$$y \approx Xw.$$

For this, we need to estimate our coefficient vector w. If our intention is to have a sparse coefficient vector w, then OMP is a suitable candidate, although it is now used in a different setting. We do not necessarily have that y is a compressed version of w, as the number of samples is generally much higher than the number of coefficients. Now, we have that $n << m$ rather than $n >> m$. Nevertheless, as we will see, the Orthogonal Matching Pursuit algorithm seems to perform very well in our setting. The algorithm now approximately solves the NP-hard problem

$$\hat{w} = \min_w ||w||_0 \text{ subject to } w \in \{w \mid ||Xw - y||_2 \leq \varepsilon\}. \tag{5.31}$$

Problem 5.31 is in fact equivalent to Problem 5.29, apart from a different notation of our variables to accomodate the linear regression setting.

Now that we have explained the origin of Orthogonal Matching Pursuit and have casted it to a regression setting, let us now discuss the inner workings of the algorithm. The pseudocode of the algorithm is given in Algorithm 4.4.

Algorithm 4.4 Original Orthogonal Matching Pursuit

Input: Data matrix $X = [\mathbf{x}_1, \dots, \mathbf{x}_d] \in \mathbb{R}^{n \times d}$, Response vector $\mathbf{y} \in \mathbb{R}^n$, Threshold ε.
Output: A coefficient vector $w \in \mathbb{R}^d$.

```
1:  $\tilde{\mathbf{x}}_j \leftarrow \mathbf{x}_j / ||\mathbf{x}_j||_2$, the normalized basis for $j = 1, ..., d$.
2:  $F^{(0)} \leftarrow \varnothing$
3:  $w^{(0)} = \mathbf{0} \in \mathbb{R}^d$
4:
5:  for $k = 1, 2, \dots$ do
6:      $i^{(k)} \leftarrow \arg\max_i |\tilde{\mathbf{x}}_i^T (Xw^{(k-1)} - \mathbf{y})|$
7:      if $\max_i |\tilde{\mathbf{x}}_i^T (Xw^{(k-1)} - \mathbf{y})| \leq \varepsilon$ then
8:          return $w^{(k-1)}$
9:      else
10:         $F^{(k)} = \{i^{(k)}\} \cup F^{(k-1)}$
11:         $w^{(k)} = \hat{w}_X \left(F^{(k)}, \mathbf{y}\right)$
12:     end if
```

```
13: end for
```

Let us explain the algorithm step-by-step. We start by initializing the set $F^{(k)}$ as the indices of w that are non-zero at iteration k. At the start, this is equal to the empty set $\varnothing$. Furthermore, $w^{(k)}$ is the coefficient vector at iteration k, which is initially the zero-vector. Furthermore, before we begin, we will normalize the columns of our data matrix X.

Now, at every iteration, we will calculate the gain of including the ith column of X as a regressor to our support set F. We verify if the added gain exceeds the threshold ε. If including the ith column of X to our regression task indeed yields enough gain, then we add the index i to our set F, and we update our w accordingly.

If this is not the case at iteration k, then even adding the most suitable column of X as a regressor does not yield the required gain. Hence, we stop the algorithm and output our vector $w^{(k-1)}$.

Casting Orthogonal Matching Pursuit to our setting.

In the previous subsection, we have shown how Orthogonal Matching Pursuit can be used in the regression setting of

$$y \approx Xw.$$

However, as you can see, Algorithm 4.4 is suitable for a coefficient vector $w \in \mathbb{R}^d$ and a response vector $y \in \mathbb{R}^n$. However, our scenario consists of a coefficient matrix $W \in \mathbb{R}^{p \times p}$ and a response matrix $\mathbf{X}_{[2:T]} \in \mathbb{R}^{p \times (T-1)}$. Hence, we require to do some modifications before we can apply OMP to our problem.

Approach 1: p independent OMP methods One approach is to do the OMP algorithm p times, one for each variable. In our setting, we have for one time series that

$$y = X_{i,2:T} \in \mathbb{R}^{T-1}, \qquad X = X_{\cdot,1:T-1} \in \mathbb{R}^{p \times T-1}, \qquad w = w_i \in \mathbb{R}^p.$$

Now, we can do this simply for all p time series, thereby getting the p columns w_i. However, we lose the dependency between the p columns. This becomes impractical later on when we also want to constrain W to adhere to a DAG. For this, we need to compare the coefficients of all columns simultaneously.

Approach 2: Cast our matrix notation to vector notation Another approach is to modify the algorithm to be applied to multiple variables at the same time. Interestingly, this can be done quite easily by some small modifications.

The conventional notation of Orthogonal Matching Pursuit is

$$\underset{w \in \mathbb{R}^p}{\arg\min} \, \|y - Xw\|_2^2 \text{ subject to } ||w||_0 \leq k, \tag{5.32}$$

whereas our desired matrix notation is

$$\underset{W \in \mathbb{R}^{p \times p}}{\arg\min} \, \left\|\mathbf{X}_{[2:T]} - \mathbf{X}_{[1:T-1]} W\right\|_F^2 \text{ subject to } ||W||_0 \leq k. \tag{5.33}$$

Unfortunately, the conventional notation in the literature is of the form of Equation 5.32. Nevertheless, we can modify the algorithms to accommodate problems of the form of Equation 5.33. However, an easier approach is to rewrite our data matrix $\mathbf{X}$ and matrix W into the form of Equation 5.32. Then, we know that the vectorized dimensions will be

$$\|y' - X'w'\|_2^2,$$

with

$$y' \in \mathbb{R}^{p \cdot (T-1)}, \qquad X' \in \mathbb{R}^{p^2 \times p \cdot (T-1)}, \qquad w' \in \mathbb{R}^{p^2}.$$

Rewrite to response vector y'. To rewrite our response matrix $\mathbf{X}_{[2:T]} \in \mathbb{R}^{(T-1)\times p}$ to a response vector $y' \in \mathbb{R}^{(T-1)\cdot p}$, We will vertically stack our $y_i \in \mathbb{R}^{T-1}$ to get a column vector $y \in \mathbb{R}^{p\cdot(T-1)}$. In mathematical notation,

$$\begin{aligned} y &= vec(y_1, y_2, \ldots, y_p) \\ &= (y_1, y_2, \ldots, y_p)^T \\ &= \left(\underbrace{X_{2,1}, X_{3,1}, \ldots, X_{T,1}}_{y_1}, \ldots, \underbrace{X_{2,p}, X_{3,p}, \ldots, X_{T,p}}_{y_p} \right)^T . \end{aligned}$$

Rewrite coefficient matrix W to coefficient vector w'. Secondly, we will vectorize our coefficient matrix $W \in \mathbb{R}^{p\times p}$ to a coefficient vector $w' \in \mathbb{R}^{p^2}$ by vertically stacking the columns $W_{\cdot,i}$. Therefore, we have

$$\begin{aligned} w' &= vec(W) \\ &= (w_1, \ldots, w_p)^T \\ &= \left(\underbrace{w_{11}, \ldots, w_{1p}}_{W_{\cdot,1}}, \ldots, \underbrace{w_{p1}, \ldots w_{pp}}_{W_{\cdot,p}} \right)^T . \end{aligned}$$

Rewrite to data matrix X'. Thirdly, we need to define our data matrix $X' \in \mathbb{R}^{p^2\times p\cdot(T-1)}$, such that

$$\mathbf{X}_{[1:T-1]} W = X' w'.$$

We achieve this by repeating the block matrix $X_{[1:T-1]} \in \mathbb{R}^{(T-1)\times p}$ along the diagonal of X' total of p times. The other entries in the matrix X' are all equal to zero. An example of rewriting X' for a certain column i OF W is given in Example 5.4.

Example 5.4 Convert ith column of W from matrix to vector form.

As an example, consider estimating W_i, the ith column of our matrix W. We want the coefficients corresponding to $i-1$ first columns to be multiplied by zero. Therefore, we we simply prepend a block of size $(i-1)\times(T-1)$ with zeros before the matrix $\mathbf{X}_{[1:T-1]}$. Similarly, we postpend a block of size $(p-i)\times(T-1)$ containing only zeros at the end of this block. For the i column, this gives us the equality

$$\left(\underbrace{\mathbf{0}, \ldots, \mathbf{0},}_{(i-1)\cdot p} \ \mathbf{X}_{[1:T-1]}, \ \underbrace{\mathbf{0}, \ldots, \mathbf{0}}_{(p-i)\cdot p} \right) w' = \mathbf{X}_{[1:T-1]} W_i.$$

This way, coefficients of W not corresponding to the ith column will be multiplied by zero, and the coefficients of the ith column will be multiplied by the data matrix $\mathbf{X}_{[1:T-1]}$. In the end, we get a block of size $p\times(T-1)$ that we use to estimate the coefficients of the ith column.

We create such a $p^2\times(T-1)$ block for all p variables, and we stack these vertically, resulting in a $p^2\times p\cdot(T-1)$ data matrix. In matrix notation, we get

$$X' = \begin{pmatrix} \mathbf{X}_{[1:T-1]} & \mathbf{O} & \cdots & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{X}_{[1:T-1]} & \cdots & \mathbf{O} & \mathbf{O} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathbf{O} & \mathbf{O} & \cdots & \mathbf{X}_{[1:T-1]} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & \cdots & \mathbf{O} & \mathbf{X}_{[1:T-1]} \end{pmatrix} \in \mathbb{R}^{p^2\times p\cdot(T-1)}.$$

A more concise mathematical notation for this using the Kronecker product is

$$X' = I_p \otimes \mathbf{X}_{[1:T-1]} \in \mathbb{R}^{p^2 \times T-1}.$$

To conclude, we see that we have rewritten our matrix sparsity problem to a vector sparsity problem:

$$\mathbf{X}_{[2:T]} - \mathbf{X}_{[1:T-1]}W \iff y' - X'w'.$$

Example 5.5 Rewrite X to vector form

To explain the mathematical formulae more concretely, suppose that we have four samples of three variables in our data matrix X. Hence, $T = 4$ and $n = 3$, and $X \in \mathbb{R}^{4x3}$. For the sake of clarity, let us assume the data matrix is defined as

$$X = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \\ 10 & 11 & 12 \end{pmatrix}.$$

Now, we have that for predicting, we use the first $T-1$ timesteps. Furthermore, we use the last $T-1$ timesteps to compare to our predictions. In the end, we get

$$X_{pred} = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}, \qquad X_{val} = \begin{pmatrix} 4 & 5 & 6 \\ 7 & 8 & 9 \\ 10 & 11 & 12 \end{pmatrix}.$$

Now, we want to estimate a matrix W such that $\|X_{val} - X_{pred}W\|_2^2$ is minimized such that the graph induced by W is a directed acyclic graph. To use OMP, we will rewrite our matrices X_{pred} and X_{val} to a matrix X' and y' respectively. First, we get y' by vectorizing X_{val}, thereby stacking the columns of X_{val}, yielding

$$y' = (4, 7, 10, 5, 8, 11, 6, 9, 12)^T \in \mathbb{R}^9.$$

Now, to get X', we repeat the block X_{pred} a total of three times along the diagonal, yielding

$$X' = \begin{pmatrix} X_{pred} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & X_{pred} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & X_{pred} \end{pmatrix}$$
$$= \begin{pmatrix} 1 & 2 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 4 & 5 & 6 & 0 & 0 & 0 & 0 & 0 & 0 \\ 7 & 8 & 9 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 2 & 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 5 & 6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 7 & 8 & 9 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4 & 5 & 6 \\ 0 & 0 & 0 & 0 & 0 & 0 & 7 & 8 & 9 \end{pmatrix} \in \mathbb{R}^{9\times 9}.$$

Now, we are looking for the nine-dimensional vector w', rather than the three-by-three dimensional matrix W such that $X'w' \approx y'$. We are now in the vector setting in which OMP is often used.

Approach 3: Modifying the OMP algorithm itself. Approach 2 suffers from the drawback that the dimensions of our data matrix X' will get unnecessarily big, and the information in X_{pred} is redundantly copied a total of p times. Furthermore, we do not utilize the information we have about structure of X', namely that a large portion of our matrix contains no information whatsoever. Therefore, it might be more practical to modify the OMP algorithm such that we can regress on a matrix of coefficients W, rather than a vector of coefficients w.

Algorithm 4.5 Matrix Orthogonal Matching Pursuit

Input: Data matrix $X = X_{pred} = [\mathbf{x}_1, \dots, \mathbf{x}_p] \in \mathbb{R}^{p\times(T-1)}$,
Response matrix $Y = X_{val} = [\mathbf{y}_1, \dots, \mathbf{y}_p] \in \mathbb{R}^{p\times(T-1)}$,
Threshold ε.
Output: A coefficient matrix $W \in \mathbb{R}^{p\times p}$.

```
1:  $\tilde{\mathbf{x}}_j \leftarrow \mathbf{x}_j / ||\mathbf{x}_j||_2$, the normalized basis for $j = 1, ..., p$.
2:  $F^{(0)} \leftarrow \varnothing$
3:  $W^{(0)} = \mathbf{O} \in \mathbb{R}^{p\times p}$
4:
5:  for $k = 1, 2, \dots$ do
6:      $i^{(k)}, j^{(k)} \leftarrow \arg\max_{i,j} \left| \tilde{\mathbf{x}}_i^T \left( \left( XW^{(k-1)} \right)_j - \mathbf{y}_j \right) \right|$
7:      if $\max_{i,j} \left| \tilde{\mathbf{x}}_i^T \left( \left( XW^{(k-1)} \right)_j - \mathbf{y}_j \right) \right| \leq \varepsilon$ then
8:          return $W^{(k-1)}$
9:      else
10:         $F^{(k)} = \left\{ \left( i^{(k)}, j^{(k)} \right) \right\} \cup F^{(k-1)}$
11:         $W^{(k)} = \texttt{OLS}\left( X_{F^{(k)}}, \mathbf{y} \right)$
12:     end if
13: end for
```

Let us consider the differences between OMP for response vectors and OMP for response matrices. Apart from some notational changes, both algorithms remain very similar. In terms of output, both algorithms return the exact same results, albeit in a different format. The only major changes are in line six and seven, where we are looking for the coefficient $W_{i,j}$ that will yield the largest gain. The index i denotes the independent variable (the $\mathbf{x}$), whereas the index j denotes the dependent variable (the $\mathbf{y}$). This way of rewriting the OMP algorithm implies that it can be easily applied to our problem setting.

Enforce DAG-ness of W.

Now that we are able to apply the Orthogonal Matching Pursuit algorithm described in Algorithm 4.5 to our problem, there is still one hurdle to overcome that is central in this thesis. The graph induced by the weighted adjacency matrix W must be a DAG. However, in its current form, Algorithm 4.5 does not enforce this. However, with greedy algorithms such as OMP, it is quite straightforward to enforce DAG-ness. At each iteration k, when we add a new coefficient or edge to our matrix W, we can first check if adding this edge will create a cycle in the graph. If this is indeed the case, then we have two options:

1. We simply stop the algorithm just before the first cycle is created.
2. We disregard the possibility of ever adding this edge, as this edge results in the smallest gain of all edges in the cycle. After this edge has been disregarded, we continue our algorithm. Everytime we encounter an edge that violates the DAG-ness of W, the possibility of ever adding this will be disregarded. The algorithm continues until all candidate edges do not yield a sufficient gain (larger than the threshold ε) or when there are only edges left that will violate the DAG-ness of W.

Distinguishing True Relations from Noise

Visual Inspection

Threshold on Edge Weight

Threshold on Gain per Edge

Validation set

Bootstrapping

Statistical Guarantees

The Mean Squared Error decreases at every iteration, unless $\max_i |\tilde{\mathbf{x}}_i^T (Xw^{(k-1)} - \mathbf{y})| = 0$.

Similar to Paper of Zhang Some statement in the form of: "Assume the assumptions of (1) hold. Then, if the threshold ϵ is larger than $x(\eta)$, we expect to recover all true coefficients with probability η.

5.3.5 LINGNAM-OLS

Perform OLS, iteratively set the non-zero coefficient that is smallest in absolute value to zero until we have a DAG.

5.3.6 LINGNAM-LASSO

Perform LASSO with regularization parameter λ, iteratively increase λ until we have a DAG.

5.4 Miscellaneous Approaches

5.4.1 Learning P^TAP with "moving" A

To quote [6]: "looking for an optimal T given a fixed P makes sense, but changing P for a fixed T does not." The entry T_{ij} originally capured the effect of $X_{P(j)}$ on $X_{P(i)}$. However, after changing the permutation matrix from P to P', T_{ij} captured the effect of $X_{P'(j)'}$ on $X_{P'(i)}$. These effects can be totally different, hence the previous estimate T_{ij} is now meaningless. However, an approach would be to also shift this matrix T_{ij} along. We are looking for a shift that after changing from P to P', the entry T_{ij} is shifted to $T_{i'j'}$, such that the estimate still remains meaningful for the specific i' and $'j'$, and that T_{ij} now contains the current estimate of $X_{P'(j)}$ on $X_{P'(i)}$. However, for computing the current cost, we will only use the lower triangular part of T, to enforce acyclity.

Chapter 6

Evaluation

This chapter evaluates the methods and the model.

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6.1 Performance Criteria

True Positive Rate.

True Negative Rate.

Precision.

Recall.

Precision-Recall Curve.

Area Under Precision-Recall Curve.

Structural Hamming Distance.

6.2 Datasets

6.2.1 Simulated Datasets

Data can be generated in multiple ways: - Hénon map. - Lorenz system. - $\mathbf{X}_t = A\mathbf{X}_{t-1} + I\epsilon_t$

6.2.2 Real Datasets

- https://www.bnlearn.com/bnrepository/ - https://webdav.tuebingen.mpg.de/cause-effect/

Chapter 7

Conclusions

This is the conclusion.

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Appendix A

Code Snippets

This Appendix contains numerous small snippets of code that were used throughout this thesis. Note that this appendix does not contain the more complicated code associated with the algorithms, but rather simple scripts that aid in the understanding of concepts described throughout this thesis. The code snippets are provided in order of appearance in the thesis, starting from the snippets used in the introduction, to the snippets used in the conclusion.

A.1 Counting the number of permutations suitable to a matrix W

```python
import numpy as np
import itertools

def get_permutations(W):
    """@params: Weighted Adjacency Matrix W as numpy array"""
    # tracks the total number of permutations
    total = 0

    # iterate over all permutations of the identity matrix
    for perm in itertools.permutations(np.identity(np.shape(W)[0])):
        # convert to numpy array
        P = np.array(perm)

        # check if we have an upper triangular matrix
        if np.allclose(P.T @ W @ P, np.triu(P.T @ W @ P)):
            total += 1

    # return the number of suitable permutations
    return total
```

Appendix B

List of datasets

List of datasets.

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Appendix C

Additional tables

The tables.

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