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Parameter Identification and  
Assessment of Independence in  
Multivariate Statistical Modeling

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A dissertation  
submitted in partial fulfillment of the  
requirements for the degree of

Doctor of Philosophy

University of Washington

2018

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Program Authorized to Offer Degree:  
Statistics

University of Washington

**Abstract**

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We are interested in the extent to which, possibly causal, relationships can be statistically quantified from multivariate data obtained from a system of random variables. In the ideal setting, we would begin with refined knowledge of which variables in our system can causally impact one another and be in the position to perform randomized controlled experiments where any intervention is possible. Unfortunately this ideal is often unrealistic: in many important cases it is impossible to conduct an intervention, we cannot ethically ask a pregnant mother to start smoking or feasibly assign a country a new governmental system, and, additionally, a researcher may have little or no prior knowledge of how their system of variables interact. This dissertation studies two problems that arise as we depart from the experimental ideal.

While scientists may not always be able to conduct a controlled experiment, thus only having observational data, they may they may be able to hypothesize or determine the directions in which causal relations point. For instance, “mother smoking during first trimester of pregnancy” may causally impact “baby birth weight” but, without time travel, certainly the reverse is impossible. Unfortunately causal relationships can be infeasible to estimate from observational data due to the presence of hidden confounding variables. In a more recent shift of paradigm, pioneered by researchers such as Judea Pearl, Jamie Robins, Don Rubin,

and Peter Spirtes, causal knowledge is represented by a directed graph whose vertices are the variables in the system. These directed graphs have a corresponding mathematical formalism called structural causal models. We consider the setting of linear structural causal models, models in which causal effects are assumed to be linear. We present combinatorial criteria for determining whether or not, given a graph, the corresponding causal relationships can be consistently estimated from observational data in the presence of hidden confounding. In particular we define determinantal instrumental variables, a generalization of the well-known instrumental variables, which can be used to identify causal effects.

Departing even further from the above ideal, a scientist may be in the exploratory stage of research and thus have little to no understanding of the causal or functional relationships in their data. In this case, a natural first question to ask is whether or not the observed variables are associated at all. That is, we would like to test whether or not the observed variables are independent. To this end, we develop a class of nonparametric measures of dependence which generalize many rank measures of association such as Kendall's  $\tau$ , Spearman's  $\rho$ , Hoeffding's  $D$ , and the more recently developed Bergsma–Dassios Sign Covariance  $\tau^*$ . This new class leads naturally to multivariate extensions of  $\tau^*$ . Our measures may be estimated unbiasedly using U-statistics, for which we prove results on computational efficiency and large-sample behavior. The algorithms we develop for their computation include, to the best of our knowledge, the first efficient algorithms for Hoeffding's  $D$  statistic in the multivariate setting.

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## ACKNOWLEDGMENTS

First and foremost I must thank my advisor Mathias Drton for his support, guidance, and passion throughout my time in graduate school. There is something deeply humbling about your ability to be both kind and brilliant in equal measure, I will miss our frequent chats on life and mathematics. I would also like to thank my committee members: Thomas, thank you for always being there when I needed feedback, questions answered, or a letter written (also for not minding all the follow up emails I sent); Marina, thank you for helping me grow as a statistician and researcher, from your machine learning course the first quarter of my graduate studies to now, you have helped me learn so much.

I could not have gotten this far without my friends, my partner Ada, and my mom Angelica, I can never hope to repay your love and support.

## DEDICATION

To my grandfather, Siegfried Weihs.

## Chapter 1

### INTRODUCTION

Multivariate analysis is the study of how data can be used to clarify relationships between random quantities. Ideally we would be in the position to interpret the associations we discover as being causal. When data has been collected from a controlled clinical trial this process is, by design, relatively straightforward. Unfortunately controlled trials can be expensive, ethically problematic, and conceptually impossible; in such cases, observational data is the only source of information from which we may make decisions. In observational data however, it is all too easy to mistake association induced by unseen confounding with the desired causal effect. Understanding when causal parameters can be consistently estimated from observational data is the problem of parameter identifiability. In the first part of this dissertation we will study the problem of parameter identifiability in the setting of linear structural causal models. Establishing parameter identifiability requires that a researcher understand the direction of causal relationships in their data, when this information is not available, in the case of data exploration for example, a first question of interest may be testing whether there is any relationship between random variables at all, this is the problem of dependence testing.

In the second part of this dissertation we will study the problem of dependence testing. In particular we develop a new class of nonparametric measures of dependence which generalize classical rank statistics of association. These measures have many desirable properties, namely they are invariant to monotonic transformations of the data, thus being robust to outliers, and often have power against all alternatives, that is, they are able to detect any dependence relationship between random variables.

In this chapter's remainder, we will give a more in depth introduction to our two problems

of interest to help situate our contributions to the literature. We will then end with a discussion of the dissertation’s organization.

### 1.1 *Parameter Identifiability in Linear Structural Causal Models*

While scientists may not understand a particular mechanism of causation, they may hypothesize or actually be able to determine its direction. For instance,  $S =$  “mother smoking during first trimester of pregnancy” may causally impact  $W =$  “baby birth weight” but the reverse is impossible. Such causal relationships are naturally depicted using directed arrows. We may faithfully model the joint distribution of  $S$  and  $W$  by letting  $S = f_S(U_S)$  and  $W = f_W(S, U_W)$  where  $f_S, f_W$  are measurable functions, and  $U_S$  and  $U_W$  are real-valued and independent (denoted by  $U_S \perp\!\!\!\perp U_W$ ). Here the *exogenous* random variables  $U_S, U_W$  contribute randomness to the *endogenous* random variables  $S, W$ . While this model places no restrictions on the joint distribution of  $(S, W)$  it comes with the implicit causal assumption that, were we to intervene by forcing a mother not to smoke ( $S = 0$ ), then  $W = f_W(0, U_W)$ . In some cases a scientist may expect that certain variables are confounded by unobserved effects. For instance, genetics could impact both whether a mother smokes and baby weight. Such confounding is graphically represented with a bidirected arrow between two vertices and, statistically, corresponds dropping the assumption that  $U_S \perp\!\!\!\perp U_W$ . The problem of *parameter identifiability* asks if causal quantities of interest, e.g.  $E[f_W(1, U_W) - f_W(0, U_W)] =$  “the average causal effect of a mother smoking on baby weight,” can be estimated from observational data.

To formalize the above intuitive description let  $G = (V, D, B)$  be a *mixed graph* where  $V$  is a set of  $|V| = d$  vertices,  $D \subset V \times V$  is a collection of *directed edges*, and  $B \subset V \times V$  is a collection of *bidirected edges*; we assume there are no self loops in  $D$  or  $B$  and that  $B$  is symmetric, that is  $(v, w) \in B$  implies  $(w, v) \in B$ . Now let  $\mathcal{F}_G$  be the collection of all tuples of measurable functions  $(f_v)_{v \in V}$  with  $f_v : \mathbb{R}^{|\text{pa}(v)|+1} \rightarrow \mathbb{R}$ . Let  $\mathcal{U}_G$  be the collection of all probability distributions  $P_U$  on  $\mathbb{R}^d$  that are Markov with respect to the bidirected edges of  $G$ ; in particular, a random vector  $U \sim P_U$  has  $U_v \perp\!\!\!\perp U_w$  whenever  $v \neq w$  and  $(v, w) \notin B$ .

Given a pair  $((f_v)_{v \in V}, P_U) \in \mathcal{F}_G \times \mathcal{U}_G$ , we may define a distribution for endogenous variables  $X = (X_v)_{v \in V}$  by setting

$$X_v := f_v(X_{pa(v)}, U_v) \quad \text{for all } v \in V,$$

for an exogenous random vector  $U = (U_v)_{v \in V} \sim P_U$ . The set of joint distributions for  $X$  obtained in this way is the *structural causal model*  $\mathcal{M}_G$ . A parameter in a structural causal model, possibly defined using interventions such as fixing a coordinate  $X_v$  to a certain value, is identifiable if it is a function of the joint distribution of the observed endogenous random variables. This dissertation will focus on *linear* structural causal models, that is the setting where all  $f_v$  are linear and  $U$  is multivariate normal. A detailed discussion of linear structural causal models and their relationships to mixed graphs is given in Chapter 2.

These linear structural causal models have direct implications for the fully nonparametric case as, if a parameter is unidentifiable under these restrictions, it must also be unidentifiable in the larger nonparametric model. In these linear models, parameter identifiability is entirely determined by the covariance matrix  $\Sigma$  of  $X$  which is parameterized as the rational function

$$\Sigma := \varphi_G(\Lambda, \Omega) := (I - \Lambda)^{-T} \Omega (I - \Lambda)^{-1}$$

where  $\Lambda = (\lambda_{vw})_{v,w \in V}$ ,  $\Omega = (\omega_{vw})_{v,w \in V}$  are  $d \times d$  matrices of indeterminants with support determined by  $D$  and  $B$  respectively. In this setting, the direct causal effect of  $X_v$  on  $X_w$  equals  $\lambda_{vw}$  and we say that  $\lambda_{vw}$  is *globally identifiable* if for any choice of  $(\Lambda, \Omega)$  we can recover  $\lambda_{vw}$  from  $\varphi_G(\Lambda, \Omega)$ . However, global identifiability is sometimes too strong a condition to require and it is also interesting to study *generic identifiability* which holds for a parameter  $\lambda_{vw}$  if we can recover  $\lambda_{vw}$  from  $\varphi_G(\Lambda, \Omega)$  for almost every choice of a pair of matrices  $(\Lambda, \Omega)$ .

Due to Wright's trek rule (Wright, 1921) questions of identifiability in a linear structural causal model can be translated into questions on the combinatorial structure of systems of paths in  $G$ . From this perspective, Foygel et al. (2012a) developed the half-trek criterion which provides necessary as well as sufficient conditions for determining generic (un)identifiability. In Chapter 3, we will show how combinatorial characterizations of sub-determinants of  $\Sigma$  (Draisma et al., 2013; Sullivant et al., 2010) can be used to substantially

improve upon the half-trek criterion. We have made these techniques easily accessible by incorporating them into the open-source R package `SEMID` (Foygel Barber et al., 2017).

## 1.2 Measuring Dependence Nonparametrically

While the Pearson correlation coefficient  $r$  is by far the most popular measure of association between random variables,<sup>1</sup> it suffers from a number of critical weaknesses. Namely the value of  $r$  can change dramatically when monotonically transforming the underlying data, a common preprocessing step, and  $r$ , being a measure of linear association, can fail to detect nonlinear relationships even with infinite samples. Given two random vectors  $X \in \mathbb{R}^r$  and  $Y \in \mathbb{R}^s$  we are interested in measures of dependence  $\mu$  which do not suffer from these weaknesses. Namely  $\mu$  should be *nonparametric*, that is invariant to any monotonic transformation of the coordinates of  $X$  and  $Y$ , and *consistent*, able to detect any relationship between  $X$  and  $Y$  so that  $\mu(X, Y) = 0$  if and only if  $X \perp\!\!\!\perp Y$ .

In Chapter 5 we will introduce *symmetric rank covariances*, a new class of dependence measures which generalize rank measures of association such as Kendall’s  $\tau$  (Kendall, 1938), Spearman’s  $\rho$  (Spearman, 1904), Hoeffding’s  $D$  (Hoeffding, 1948), and recently developed Bergsma–Dassios Sign Covariance  $\tau^*$  (Bergsma and Dassios, 2014). Symmetric rank covariances are nonparametric and we identify special cases which are also consistent. For these symmetric rank covariances we prove results on computational efficiency (Chapter 6), large-sample behavior (Chapter 7), and empirically compare our measures against other contemporaries such as the distance covariance of Székely et al. (2007). Software to perform inference and tests with symmetric rank covariances is available in the open source packages `TauStar` (Weihs, 2015) and `SymRC` (Weihs, 2018).

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<sup>1</sup>At the time of writing, a Google search for “Pearson correlation” has  $\sim 30$  times more results than the next most popular dependence measure considered in this manuscript, the second being the distance covariance of Székely et al. (2007) with  $\sim 2.5$  million results.

### ***1.3 Organization***

This dissertation is organized in two parts, each with multiple chapters. The first part discusses work on the problem of parameter identifiability in linear structural causal models while the second provides our contributions to nonparametric measures of dependence. Throughout this work, proofs will often be moved to appendices found at the end of their corresponding parts.

Part I

**PARAMETER IDENTIFIABILITY IN  
LINEAR STRUCTURAL CAUSAL MODELS**

## Chapter 2

### INTRODUCTION AND PRELIMINARIES

In a *linear structural causal model* the joint distribution of a random vector  $X = (X_1, \dots, X_n)^T$  obeys noisy linear interdependencies. These interdependencies can be expressed with a matrix equation of the form

$$X = \lambda_0 + \Lambda^T X + \epsilon, \quad (2.1)$$

where  $\Lambda = (\lambda_{vw}) \in \mathbb{R}^{n \times n}$  and  $\lambda_0 = (\lambda_{01}, \dots, \lambda_{0n})^T \in \mathbb{R}^n$  are unknown parameters, and  $\epsilon = (\epsilon_1, \dots, \epsilon_n)^T$  is a random vector of error terms with positive definite covariance matrix  $\Omega = (\omega_{vw})$ . Here  $X$  has mean vector  $(I - \Lambda)^{-T} \lambda_0$  and covariance matrix

$$\varphi(\Lambda, \Omega) := (I - \Lambda)^{-T} \Omega (I - \Lambda)^{-1} = \Sigma \quad (2.2)$$

where  $I$  is the  $n \times n$  identity matrix. Linear structural equation models have been widely applied in a variety of settings due to the clear causal interpretation of their parameters (Bollen, 1989; Spirtes et al., 2000; Pearl, 2009).

Following an approach that dates back to Wright (1921, 1934), we may view  $\Lambda$  and  $\Omega$  as (weighted) adjacency matrices corresponding to directed and bidirected graphs, respectively. This yields a natural correspondence between linear structural causal models and *mixed graphs*, that is, graphs with both directed edges,  $v \rightarrow w$ , and bidirected edges,  $v \leftrightarrow w$ . More precisely, the mixed graph  $G$  is associated to the linear structural causal model in which  $\lambda_{vw}$  is assumed to be zero if  $v \rightarrow w \notin G$  and, similarly,  $\omega_{vw} = 0$  when  $v \leftrightarrow w \notin G$ . We write  $\varphi_G$  for the map obtained by restricting the map  $\varphi$  from (2.2) to pairs  $(\Lambda, \Omega)$  that satisfy the conditions encoded by the graph  $G$ . We note that mixed graphs used to represent linear structural equation models are often also called *path diagrams*.

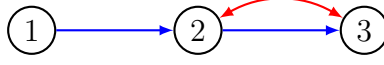


Figure 2.1: The mixed graph for the instrumental variable model.

**Example 2.1.** The mixed graph in Figure 2.1 corresponds to the well-known instrumental variable model (Didelez et al., 2010). In equations, this model asserts that

$$X_1 = \lambda_{01} + \epsilon_1, \quad X_2 = \lambda_{02} + \lambda_{12}X_1 + \epsilon_2, \quad \text{and} \quad X_3 = \lambda_{03} + \lambda_{23}X_2 + \epsilon_3,$$

where  $\epsilon$  has 0 mean and covariance matrix

$$\Omega = \begin{pmatrix} \omega_{11} & 0 & 0 \\ 0 & \omega_{22} & \omega_{23} \\ 0 & \omega_{23} & \omega_{33} \end{pmatrix}.$$

In this model, the random vector  $X = (X_1, X_2, X_3)$  has covariance matrix

$$\begin{aligned} \Sigma &= \begin{pmatrix} 1 & -\lambda_{12} & 0 \\ 0 & 1 & -\lambda_{23} \\ 0 & 0 & 1 \end{pmatrix}^{-T} \begin{pmatrix} \omega_{11} & 0 & 0 \\ 0 & \omega_{22} & \omega_{23} \\ 0 & \omega_{23} & \omega_{33} \end{pmatrix} \begin{pmatrix} 1 & -\lambda_{12} & 0 \\ 0 & 1 & -\lambda_{23} \\ 0 & 0 & 1 \end{pmatrix}^{-1} \\ &= \begin{pmatrix} \omega_{11} & \lambda_{12}\omega_{11} & \lambda_{12}\lambda_{23}\omega_{11} \\ \lambda_{12}\omega_{11} & \omega_{11}\lambda_{12}^2 + \omega_{22} & \lambda_{23}\omega_{11}\lambda_{12}^2 + \lambda_{23}\omega_{22} + \omega_{23} \\ \lambda_{12}\lambda_{23}\omega_{11} & \lambda_{23}\omega_{11}\lambda_{12}^2 + \lambda_{23}\omega_{22} + \omega_{23} & \omega_{33} + 2\omega_{23}\lambda_{23} + \lambda_{23}^2\omega_{22} \end{pmatrix}. \end{aligned}$$

A first question that arises when specifying a linear structural equation model via a mixed graph  $G$  is whether the map  $\varphi_G$  is injective, that is, whether any  $(\Lambda, \Omega)$  in the domain of  $\varphi_G$  can be uniquely recovered from the covariance matrix  $\varphi_G(\Lambda, \Omega)$ . When this injectivity holds we say that the model and associated mixed graph are *globally identifiable*. Whether or not global identifiability holds can be decided in polynomial time (Drton et al., 2011; Shpitser and Pearl, 2006; Tian and Pearl, 2002). However, in many cases global identifiability is too strong a condition. Indeed, the above instrumental variable model is not globally identifiable.

We will be instead interested in *generic identifiability*, that is, whether  $(\Lambda, \Omega)$  can be recovered from  $\varphi_G(\Lambda, \Omega)$  with probability 1 when choosing  $(\Lambda, \Omega)$  from any continuous distribution on the domain of  $\varphi_G$ . A current state-of-the-art, polynomial time verifiable, criterion for checking generic identifiability of a given mixed graph is the *half-trek criterion* of Foygel et al. (2012a), with generalizations by Chen et al. (2014); Chen (2015); Drton and Weihs (2016). The sufficient condition of the half-trek criterion operates by iteratively discovering invertible linear equation systems in the  $\Lambda$  parameters which it uses to prove generic identifiability. A necessary condition given by the half-trek criterion detects cases in which the Jacobian matrix of  $\varphi_G$  fails to attain full column rank which implies that the parameterization  $\varphi_G$  is generically infinite-to-one. However, there remain a considerable number of cases in which the half-trek criterion remains inconclusive, that is, the graph satisfies the necessary but not the sufficient condition for generic identifiability.

We extend the applicability of the half-trek criterion in two ways. First, we show how the theorems on trek separation by Sullivan et al. (2010) can be used to discover determinantal relations that in turn can be used to prove the generic identifiability of individual edge coefficients in linear structural causal models. This method generalizes the use of conditional independence in known instrumental variable techniques; compare e.g. Brito and Pearl (2002). Once we have shown that individual edges are generically identifiable with this new method, it would be ideal if identified edges could be integrated into the equation systems discovered by the half-trek criterion to prove that even more edges are generically identifiable. Unfortunately, the half-trek criterion is not well suited to integrate single edge identifications as it operates simultaneously on all edges incoming to a given node. Our second contribution resolves this issue by providing an *edgewise* half-trek criterion which operates on subsets of a node's parents, rather than all parents at once. This edgewise criterion alone often shows many more coefficients are generically identifiable than the usual half-trek criterion. In the process of preparing this work for publication we discovered the independent work of Chen (2016); as is clarified in Remark 3.11, some of our results can be seen as a generalization of results in his work.

In preparation for Chapter 3 where we present our contributions, the rest of this chapter is dedicated to formally introducing mixed graphs, the problem of generic identifiability, and the half-trek criterion.

## 2.1 Mixed Graphs and Linear Structural Causal Models

We assume some familiarity with the graphical representation of structural causal models and only give a brief overview of our objects of study. A more in-depth introduction can be found, for example, in Pearl (2009) or, with a focus on the linear case considered here, in Drton (2016). Nonzero covariances in a linear structural causal model may arise through direct or confounding effects. Mixed graphs with two types of edges have been used to represent these two sources of dependences.

**Definition 2.2** (Mixed Graph). A *mixed graph* on  $n$  vertices is a triple  $G = (V, D, B)$  where  $V = \{1, \dots, n\}$  is the vertex set,  $D \subset V \times V$  are the directed edges, and  $B \subset V \times V$  are the bidirected edges. We require that there be no self-loops, so  $(v, v) \notin D, B$  for all  $v \in V$ . If  $(v, w) \in D$ , we will write  $v \rightarrow w \in G$  and if  $(v, w) \in B$ , we will write  $v \leftrightarrow w \in G$ . As bidirected edges are symmetric we will also require that  $B$  is symmetric, so that  $(v, w) \in B \iff (w, v) \in B$ .

Let  $v$  and  $w$  be two vertices of a mixed graph  $G = (V, D, B)$ . A *path* from  $v$  to  $w$  is any sequence of edges from  $D$  or  $B$  beginning at  $v$  and ending at  $w$ . Here, we allow that directed edges be traversed against their natural direction (i.e., from head to tail). We also allow repeated vertices on a path. Sometimes, such paths are referred to as walks or semi-walks. A path from  $v$  to  $w$  is *directed* if all of its edges are directed and point in the same direction, away from  $v$  and towards  $w$ .

**Definition 2.3** (Treks and half-treks). (a) A path  $\pi$  from a *source*  $v$  to a *target*  $w$  is a *trek*

if it has no colliding arrowheads, that is,  $\pi$  is of the form

$$v = z_l^L \leftarrow z_{l-1}^L \leftarrow \cdots \leftarrow z_1^L \longleftrightarrow z_1^R \rightarrow \cdots \rightarrow z_{r-1}^R \rightarrow z_r^R = w \quad \text{or} \quad (2.3)$$

$$v = z_l^L \leftarrow z_{l-1}^L \leftarrow \cdots \leftarrow z_1^L \leftarrow z^T \rightarrow z_1^R \rightarrow \cdots \rightarrow z_{r-1}^R \rightarrow z_r^R = w, \quad (2.4)$$

where  $z^T$  is called the *top node*. Each trek  $\pi$  has a left-hand side  $\text{Left}(\pi)$  and a right-hand side  $\text{Right}(\pi)$ . In (2.3),  $\text{Left}(\pi) = \{z_1^L, \dots, z_l^L\}$  and  $\text{Right}(\pi) = \{z_1^R, \dots, z_r^R\}$ . In (2.4),  $\text{Left}(\pi) = \{z^T, z_1^L, \dots, z_l^L\}$  and  $\text{Right}(\pi) = \{z^T, z_1^R, \dots, z_r^R\}$ , with  $z^T$  a part of both sides.

(b) A trek  $\pi$  is a *half-trek* if  $|\text{Left}(\pi)| = 1$ . In this case  $\pi$  is of the form

$$z_1^L \longleftrightarrow z_1^R \rightarrow \cdots \rightarrow z_r^R \quad \text{or} \quad z^T \rightarrow z_1^R \rightarrow \cdots \rightarrow z_r^R.$$

In particular, a half-trek from  $v$  to  $w$  is a trek from  $v$  to  $w$  which is either empty, begins with a bidirected edge, or begins with a directed edge pointing away from  $v$ .

Some terminology is needed to reference the local neighborhood structure of a vertex  $v$ . For the directed part  $(V, D)$  of the mixed graph, it is standard to define the set of *parents* and the set of *descendants* of  $v$  as

$$\text{pa}(v) = \{w \in V : w \rightarrow v \in G\},$$

$$\text{des}(v) = \{w \in V : \exists \text{ a non-empty directed path from } v \text{ to } w \text{ in } G\},$$

respectively. The nodes incident to a bidirected edge can be thought of as having a common (latent) parent and thus we refer to the bidirected neighbors as *siblings* and define

$$\text{sib}(v) = \{w \in V : w \leftrightarrow v \in G\}.$$

Finally, we denote the sets of nodes that are *trek reachable* or *half-trek reachable* from  $v$  by

$$\text{tr}(v) = \{w \in V : \exists \text{ a non-empty trek from } v \text{ to } w \text{ in } G\},$$

$$\text{htr}(v) = \{w \in V : \exists \text{ a non-empty half-trek from } v \text{ to } w \text{ in } G\}.$$

Two sets of matrices may be associated with a given mixed graph  $G = (V, D, B)$ . First,  $\mathbb{R}_{\text{reg}}^D$  is the set of real  $n \times n$  matrices  $\Lambda = (\lambda_{vw})$  with support  $D$ , i.e., those matrices  $\Lambda$  with

$\lambda_{vw} \neq 0$  implying  $v \rightarrow w \in G$  and for which  $I - \Lambda$  invertible. Second,  $PD(B)$  is the set of positive definite matrices with support  $B$ , i.e.,  $\omega_{vw} \neq 0$  implies either  $v = w$  or  $v \leftrightarrow w \in G$ . Based on (2.2), the distributions in the linear structural causal model given by  $G$  have a covariance matrix  $\Sigma$  that is parameterized by the map

$$\varphi_G : (\Lambda, \Omega) \mapsto (I - \Lambda)^{-T} \Omega (I - \Lambda)^{-1} \quad (2.5)$$

with domain  $\Theta := \mathbb{R}_{\text{reg}}^D \times PD(B)$ .

*Remark 2.4.* Our focus is solely on covariance matrices. Indeed, in the traditional case where the errors  $\epsilon$  in (2.1) follow a multivariate normal distribution the covariance matrix contains all available information about the parameters  $(\Lambda, \Omega)$ .

Subsequently, the matrices  $\Lambda, \Omega$  and  $\Sigma$  will also be regarded as matrices of indeterminants. The entries of  $(I - \Lambda)^{-1} = I + \sum_{k=1}^{\infty} \Lambda^k$  may then be interpreted as formal power series. Let  $\Lambda$  and  $\Omega$  be matrices of indeterminants with zero pattern corresponding to  $G$ . Then  $\Sigma = \varphi_G(\Lambda, \Omega)$  has entries that are formal power series whose form is described by the Trek Rule of Wright (1921), see also Spirtes, Glymour, and Scheines (2000). The Trek rule states that for every  $v, w \in V$  the corresponding entry of  $\varphi_G(\Lambda, \Omega)$  is the sum of all trek monomials corresponding to treks from  $v$  to  $w$ .

**Definition 2.5** (Trek Monomial). Let  $v, w \in V$  be two, not necessarily distinct, vertices, and let  $\mathcal{T}(v, w)$  be the set of all treks from  $v$  to  $w$  in  $G$ . If  $\pi \in \mathcal{T}(v, w)$  contains no bidirected edge and has top node  $z$ , its *trek monomial* is defined as

$$\pi(\Lambda, \Omega) = \omega_{zz} \prod_{x \rightarrow y \in \pi} \lambda_{xy}.$$

If  $\pi$  contains a bidirected edge connecting  $u, z \in V$ , then its trek monomial is

$$\pi(\Lambda, \Omega) = \omega_{uz} \prod_{x \rightarrow y \in \pi} \lambda_{xy}.$$

**Proposition 2.6** (Trek Rule). *The covariance matrix  $\Sigma = \varphi_G(\Lambda, \Omega)$  corresponding to a mixed graph  $G$  satisfies*

$$\Sigma_{vw} = \sum_{\pi \in \mathcal{T}(v,w)} \pi(\Lambda, \Omega), \quad v, w \in V.$$

## 2.2 Generic Identifiability

We now formally introduce our problem of interest and review relevant prior work. We recall that an *algebraic set* is the zero-set of a collection of polynomials. An algebraic set that is a proper subset of Euclidean space has measure zero; see, e.g., the lemma in Okamoto (1973).

**Definition 2.7** (Generic Identifiability). (a) The model given by a mixed graph  $G$  is *generically identifiable* if there exists a proper algebraic subset  $A \subset \Theta$  such that the *fiber*  $\mathcal{F}(\Lambda, \Omega) := \varphi_G^{-1}(\{\varphi_G(\Lambda, \Omega)\})$  is a singleton set, that is, it satisfies

$$\mathcal{F}(\Lambda, \Omega) = \{(\Lambda, \Omega)\}$$

for all  $(\Lambda, \Omega) \in \Theta \setminus A$ . That is,  $\varphi_G$  should be injective when restricted to the set  $\Theta \setminus A$ . In this case we will say, for simplicity, that  $G$  is generically identifiable.

(b) Let  $\text{proj}_{v \rightarrow w}$  be the projection  $(\Lambda, \Omega) \mapsto \lambda_{vw}$  for  $v \rightarrow w \in G$ . We say that the edge coefficient  $\lambda_{vw}$  is *generically identifiable* if there exists a proper algebraic subset  $A \subset \Theta$  such that  $\text{proj}_{v \rightarrow w}(\mathcal{F}(\Lambda, \Omega)) = \{\lambda_{vw}\}$  for all  $(\Lambda, \Omega) \in \Theta \setminus A$ . In this case, we will say that the edge  $v \rightarrow w$  is generically identifiable.

In all examples we know of, if generic identifiability holds, then the parameters can in fact be recovered using rational formulas.

**Definition 2.8** (Rational Identifiability). (a) A mixed graph  $G$ , or rather the model it defines, is *rationally identifiable* if there exists a rational map  $\psi$  and a proper algebraic subset  $A \subset \Theta$  such that  $\psi \circ \varphi_G$  is the identity on  $\Theta \setminus A$ .

(b) An edge  $v \rightarrow w \in G$ , or rather the coefficient  $\lambda_{vw}$ , is *rationally identifiable* if there exists a rational function  $\psi$  and a proper algebraic subset  $A \subset \Theta$  such that  $\psi \circ \varphi_G(\Lambda, \Omega) = \lambda_{vw}$  for all  $(\Lambda, \Omega) \in \Theta \setminus A$ .

We now introduce the half-trek criterion (HTC) of Foygel et al. (2012a). We generalize this criterion in Section 3.2. The half-trek criterion operates by building systems of linear equations in the  $\Lambda$  parameters, to show that these systems are invertible requires that collections of treks do not intersect in the following sense.

**Definition 2.9** (Trek and Half-Trek Systems). Let  $\Pi = \{\pi_1, \dots, \pi_m\}$  be a collection of treks in  $G$  and let  $S, T$  be the set of sources and targets of the  $\pi_i$  respectively. Then we say that  $\Pi$  is a *system of treks* from  $S$  to  $T$ . If each  $\pi_i$  is a half-trek, then  $\Pi$  is a *system of half-treks*. A collection  $\Pi = \{\pi_1, \dots, \pi_m\}$  of treks is said to have *no sided intersection* if

$$\text{Left}(\pi_i) \cap \text{Left}(\pi_j) = \emptyset = \text{Right}(\pi_i) \cap \text{Right}(\pi_j), \quad \forall i \neq j.$$

As our focus will be on the identification of individual edges in  $G$  we do not state the identifiability result of Foygel et al. (2012a) in its usual form, instead we present a slightly modified version which is implied by the proof of Theorem 1 in Foygel et al. (2012a).

**Definition 2.10.** A set of nodes  $Y \subset V$  satisfies the *half-trek criterion* with respect to a vertex  $v \in V$  if

- (i)  $|Y| = |\text{pa}(v)|$ ,
- (ii)  $Y \cap (\{v\} \cup \text{sib}(v)) = \emptyset$ , and
- (iii) there is a system of half-treks with no sided intersection from  $Y$  to  $\text{pa}(v)$ .

**Theorem 2.11** (HTC-identifiability). *Suppose that in the mixed graph  $G = (V, D, B)$  the set  $Y \subset V$  satisfies the half-trek criterion with respect to  $v \in V$ . If all directed edges  $u \rightarrow y \in G$  with head  $y \in \text{htr}(v) \cap Y$  are generically (rationally) identifiable, then all directed edges with  $v$  as a head are generically (rationally) identifiable.*

The sufficient condition for rational identifiability of  $G$  in Foygel et al. (2012a) is obtained through iterative application of Theorem 2.11.

## Chapter 3

### DETERMINANTAL INSTRUMENTAL VARIABLES

In this chapter we will present our contributions to the problem of generic identifiability in linear structural equation models. In particular, in Section 3.1 we show how trek-separation, a refined combinatorial condition for the separation of nodes in a mixed graph introduced by Sullivant et al. (2010), allows the generic identification of edge coefficients as quotients of subdeterminants. We then introduce the edgewise half-trek criterion in Section 3.2 and we discuss necessary conditions for the generic identifiability of edge coefficients in Section 3.3. Computational experiments showing the applicability of our sufficient conditions follow in Section 3.4, and we finish with a brief conclusion in Section 3.5. Some longer proofs are deferred to Appendix A.

#### **3.1 Trek Separation and Identification by Ratios of Determinants**

Let  $\Lambda$  and  $\Omega$  be matrices of indeterminates corresponding to a mixed graph  $G = (V, D, B)$  as specified in Section 2.1. Let  $S, T \subset V$ , and let  $\Sigma_{S,T}$  be the submatrix of  $\Sigma = \varphi_G(\Lambda, \Omega) \in \mathbb{R}^{n \times n}$  obtained by retaining only the rows and columns indexed by  $S$  and  $T$ , respectively. The (generic) rank of such a submatrix  $\Sigma_{S,T}$  can be completely characterized by considering the trek systems between the vertices in  $S$  and  $T$ . The formal statement of this result follows.

**Definition 3.1** (t-separation). A pair of sets  $(L, R)$  with  $L, R \subset V$  *t-separates* the sets  $S, T \subset V$  if every trek between a vertex  $s \in S$  and a vertex  $t \in T$  intersects  $L$  on the left or  $R$  on the right.

In this definition, the symbols  $L$  and  $R$  are chosen to suggest left and right. Similarly,  $S$  and  $T$  are chosen to indicate sources and targets, respectively.

**Theorem 3.2** (Sullivant et al. (2010), Draisma et al. (2013)). *Let  $r$  be a non-negative integer. The submatrix  $\Sigma_{S,T}$  has generic rank  $\leq r$  if and only if there exist sets  $L, R \subset V$  with  $|L| + |R| \leq r$  such that  $(L, R)$   $t$ -separates  $S$  and  $T$ .*

Theorem 2.7 of Sullivant et al. (2010) established this result for acyclic mixed graphs while Draisma et al. (2013) extended the result to all mixed graphs and even gave an explicit representation of the rational form of the subdeterminant  $|\Sigma_{S,T}|$ , for  $|S| = |T|$ . An immediate corollary to the above theorem, considering the proof of Theorem 2.17 in Sullivant et al. (2010), rephrases its statement in terms of maximum flows in a certain graph. For an introduction to maximum flow, and the well-known Max-flow Min-cut Theorem, see the book by Cormen et al. (2009). Note that standard max-flow min-cut framework does not allow vertices to have maximum capacities or for there to be multiple sources and targets, introducing these modifications is, however, trivial and the resulting theorem is sometimes called the Generalized Max-flow Min-cut Theorem.

**Corollary 3.3.** *Let  $G_{\text{flow}} = (V_f, D_f)$  be the directed graph with  $V_f = \{1, \dots, n\} \cup \{1', \dots, n'\}$  and  $D_f$  containing the following edges:*

$$i \rightarrow j \quad \text{if } j \rightarrow i \in G, \tag{3.1}$$

$$i \rightarrow i' \quad \text{for all } i \in V, \tag{3.2}$$

$$i \rightarrow j' \quad \text{if } i \leftrightarrow j \in G, \quad \text{and} \tag{3.3}$$

$$i' \rightarrow j' \quad \text{if } i \rightarrow j \in G. \tag{3.4}$$

*Turn  $G_{\text{flow}}$  into a flow network by giving all vertices and edges capacity 1. Let  $S = \{s_1, \dots, s_k\}$ ,  $T = \{t_1, \dots, t_m\} \subset V$ . Then  $\Sigma_{S,T}$  has generic rank  $r$  if and only if the max-flow from  $s_1, \dots, s_k$  to  $t'_1, \dots, t'_m$  in  $G_{\text{flow}}$  is  $r$ .*

*Proof.* Add vertices  $s, t$ , with infinite capacity, to the graph  $G_{\text{flow}}$  along with edges, all with capacity 1,  $s \rightarrow s_i$ , for  $1 \leq i \leq k$ , and  $t'_j \rightarrow t$ , for  $1 \leq j \leq m$ . Let  $L, R$  be such that they  $t$ -separate the sets  $S, T$  and  $|L| + |R|$  is minimal. By Theorem 3.2,  $\Sigma_{S,T}$  has rank  $|L| + |R|$

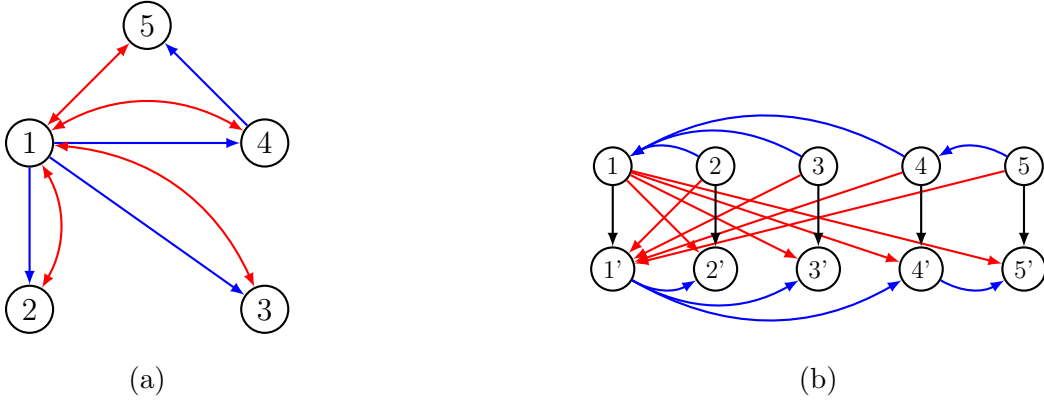


Figure 3.1: (a) A graph  $G$  that is generically identifiable but for which the HTC fails to identify any coefficients. (b) The corresponding flow graph  $G_{\text{flow}}$ , black edges correspond to (3.2), red edges to (3.3), and blue edges to (3.1) and (3.4).

generically. Now  $L \cup R$  gives the minimal size  $s-t$  cut (of size  $|L| + |R|$ ). By the (generalized) Max-flow Min-cut theorem the max-flow from  $s$  to  $t$  is  $|L| + |R|$ , and it is also the max flow from  $s_1, \dots, s_k$  to  $t'_1, \dots, t'_m$ . Hence  $\Sigma_{S,T}$  has generic rank equal to the max-flow.  $\square$

Note that the maximum flow between vertex sets in a graph can be computed in polynomial time. Indeed the conditions of Corollary 3.3 can be checked in  $O(|V|^2 \max\{m, k\})$  time (Cormen et al., 2009, page 725). As the following example shows, Corollary 3.3 can be used to find determinantal constraints on  $\Sigma$ . These constraints can then be leveraged to identify edges in  $G$ .

**Example 3.4.** Consider the mixed graph  $G = (V, D, B)$  in Figure 3.1a, which is taken from Figure 3c in Foygel et al. (2012a). The corresponding flow network  $G_{\text{flow}}$  is shown in Figure 3.1b. From Gröbner basis computations (see García-Puente et al. (2010) for an introduction to the use of computer algebra for proving rational parameter identifiability),  $G$  is known to be rationally identifiable but the half-trek criterion fails to certify that any edge of  $G$  is generically identifiable. Let  $S = \{1, 2, 4\}$  and  $T = \{1, 3, 5\}$ . Corollary 3.3 implies that  $\Sigma_{S,T}$  has generically full rank as there is a flow of size 3 from  $S$  to  $T' = \{1', 3', 5'\}$  in  $G_{\text{flow}}$ , via the

paths  $1 \rightarrow 3'$ ,  $2 \rightarrow 1'$ , and  $4 \rightarrow 5'$ . Now suppose that we remove the  $4 \rightarrow 5$  edge from  $G$ , call the resulting graph  $\bar{G}$ , and let  $\bar{\Sigma}$  be the covariance matrix corresponding to  $\bar{G}$ . Then one may check that the max-flow from  $S$  to  $T'$  in  $\bar{G}_{\text{flow}}$  is  $\leq 2$ . Thus  $|\bar{\Sigma}_{\{1,2,4\},\{1,3,5\}}| = 0$  where  $|\cdot|$  denotes the determinant. Now note that  $\lambda_{45}\sigma_{14}$  is the sum of all monomials given by treks from 1 to 5 that end in the edge  $\lambda_{45}$ . Hence,  $\sigma_{15} - \lambda_{45}\sigma_{14}$  is obtained by summing over all treks from 1 to 5 that do not end in the edge  $4 \rightarrow 5$ . But in our graph this is just the sum over treks from 1 to 5 that do not use the edge  $4 \rightarrow 5$  at all. Therefore,  $\bar{\sigma}_{15} = \sigma_{15} - \lambda_{45}\sigma_{14}$ . Similarly, it is straightforward to check that

$$\bar{\Sigma}_{\{1,2,4\},\{1,3,5\}} = \begin{pmatrix} \sigma_{11} & \sigma_{13} & \sigma_{15} - \lambda_{45}\sigma_{14} \\ \sigma_{21} & \sigma_{23} & \sigma_{25} - \lambda_{45}\sigma_{24} \\ \sigma_{41} & \sigma_{43} & \sigma_{45} - \lambda_{45}\sigma_{44} \end{pmatrix}. \quad (3.5)$$

By the multilinearity of the determinant, we deduce that

$$\begin{aligned} 0 = |\bar{\Sigma}_{\{1,2,4\},\{1,3,5\}}| &= \begin{vmatrix} \sigma_{11} & \sigma_{13} & \sigma_{15} \\ \sigma_{21} & \sigma_{23} & \sigma_{25} \\ \sigma_{41} & \sigma_{43} & \sigma_{45} \end{vmatrix} - \lambda_{45} \begin{vmatrix} \sigma_{11} & \sigma_{13} & \sigma_{14} \\ \sigma_{21} & \sigma_{23} & \sigma_{24} \\ \sigma_{41} & \sigma_{43} & \sigma_{44} \end{vmatrix} \\ &= |\Sigma_{\{1,2,4\},\{1,3,5\}}| - \lambda_{45} |\Sigma_{\{1,2,4\},\{1,3,4\}}|. \end{aligned}$$

Applying Corollary 3.3 a final time, we recognize that  $|\Sigma_{\{1,2,4\},\{1,3,4\}}|$  is generically non-zero and, thus, the equation

$$\lambda_{45} = \frac{|\Sigma_{\{1,2,4\},\{1,3,5\}}|}{|\Sigma_{\{1,2,4\},\{1,3,4\}}|}$$

generically and rationally identifies  $\lambda_{45}$ . In this case, the same strategy can be used to identify the edges  $1 \rightarrow 2$  and  $1 \rightarrow 3$  (but not  $1 \rightarrow 4$ ) in  $G$ .

In the above example, there is a correspondence between trek systems in  $G$  and trek systems in  $\bar{G}$ , the graph that has the edge to be identified removed. This allowed us to leverage Corollary 3.3 directly to show that (3.5) has determinant 0. Such a correspondence cannot always be obtained but exists in the following case.

**Theorem 3.5.** *Let  $G = (V, D, B)$  be a mixed graph. Let  $w_0 \rightarrow v$  be an edge in  $G$ , and suppose that the edges  $w_1 \rightarrow v, \dots, w_\ell \rightarrow v \in G$  are known to be generically (rationally) identifiable. Let  $\bar{G}$  be the subgraph of  $G$  with the edges  $w_0 \rightarrow v, \dots, w_\ell \rightarrow v \in G$  removed. Suppose there are sets  $S \subset V \setminus \{v\}$ ,  $T \subset V \setminus \{v, w_0\}$  with  $|S| = |T| + 1 = k$  such that:*

(a)  $\text{des}(v) \cap (S \cup T \cup \{v\}) = \emptyset$ ,

(b) *the max-flow from  $S$  to  $T' \cup \{w'_0\}$  in  $G_{\text{flow}}$  equals  $k$ , and*

(c) *the max-flow from  $S$  to  $T' \cup \{v'\}$  in  $\bar{G}_{\text{flow}}$  is less than  $k$ .*

*Then  $w_0 \rightarrow v$  is generically (rationally) identifiable by the equation*

$$\lambda_{w_0 v} = \frac{|\Sigma_{S, T \cup \{v\}}| - \sum_{i=1}^{\ell} \lambda_{w_i v} |\Sigma_{S, T \cup \{w_i\}}|}{|\Sigma_{S, T \cup \{w_0\}}|}. \quad (3.6)$$

*Proof.* Let  $\Sigma$  and  $\bar{\Sigma}$  be the covariance matrices corresponding to  $G$  and  $\bar{G}$ , respectively. Since  $\text{des}(v) \cap (S \cup T \cup \{v\}) = \emptyset$ , we have that  $\sigma_{st} = \bar{\sigma}_{st}$  for all  $s \in S$  and  $t \in T$ . This holds as, if a trek from  $s$  to  $t$  uses an edge  $w_i \rightarrow v$ , then either  $s \in \{v\} \cup \text{des}(v)$  or  $t \in \{v\} \cup \text{des}(v)$ , violating our assumptions.

Now let  $s \in S$  and  $0 \leq i \leq \ell$ . Suppose that  $\pi$  is a trek from  $s$  to  $v$  that uses the edge  $w_i \rightarrow v$ . Then since  $s \notin \{v\} \cup \text{des}(v)$  we must have that  $w_i \rightarrow v$  is used only on the right-hand side of  $\pi$ . With  $v \notin \text{des}(v)$  it follows that  $w_i \rightarrow v$  is the last edge used in the trek because  $\pi$  may only use directed edges after using  $w_i \rightarrow v$  and must end at  $v$ . Hence, all treks from  $s$  to  $v$  which use  $w_i \rightarrow v$  must have this edge as their last edge on the right. But  $\sigma_{sv} \lambda_{w_i v}$  is obtained by summing over all treks from  $s$  to  $v$  which end in the edge  $w_i \rightarrow v$  and, thus,  $\sigma_{sv} - \sigma_{sw_i} \lambda_{w_i v}$  is the sum of the monomials for all treks from  $s$  to  $v$  that do not use the  $w_i \rightarrow v$  edge at all.

As the above argument holds for all  $0 \leq i \leq \ell$ , it follows that  $\bar{\sigma}_{sv} = \sigma_{sv} - \sum_{i=0}^k \sigma_{sw_i} \lambda_{w_i v}$ . Since this is true for all  $s \in S$  it follows, similarly as in Example 3.4, that

$$|\bar{\Sigma}_{S, T \cup \{v\}}| = |\Sigma_{S, T \cup \{v\}}| - \sum_{i=0}^k \lambda_{w_i v} |\Sigma_{S, T \cup \{w_i\}}|.$$

Using assumption (c) and applying Corollary 3.3, we have  $|\bar{\Sigma}_{S,T \cup \{v\}}| = 0$ . Similarly, by assumption (b),  $|\Sigma_{S,T \cup \{w_0\}}| \neq 0$  generically. The desired result follows.  $\square$

*Remark 3.6.* Theorem 3.5 generalizes the ideas underlying instrumental variable methods such as those discussed in Brito and Pearl (2002). Indeed, this prior work uses d-separation as opposed to t-separation. D-separation characterizes conditional independence which in the present context corresponds to the vanishing of particular almost principal determinants of the covariance matrix. In contrast, Theorem 3.5 allows us to leverage arbitrary determinantal relations; compare Sullivant et al. (2010). The graph in Figure 3.1a is an example in which d-separation and traditional instrumental variable techniques cannot explain the rational identifiability of the coefficient for edge  $4 \rightarrow 5$ .

While assumption (a) in the above Theorem allows for the easy application of Corollary 3.3, this assumption can be relaxed by generalizing one direction of Corollary 3.3. We state this generalization as the following lemma, which is concerned with asymmetric treatment of edges that appear on the left versus right-hand side of treks. The lemma's proof is deferred to Appendix A .

**Lemma 3.7.** *Let  $G = (V, D, B)$  be a mixed graph, and let  $\Lambda = (\lambda_{uv})$  and  $\Omega$  be the matrices of indeterminants corresponding to the directed and the bidirected part of  $G$ , respectively. Let  $D_L, D_R \subset D$  and define  $n \times n$  matrices  $\Lambda^L$  and  $\Lambda^R$  with*

$$\Lambda_{uv}^L = \begin{cases} \lambda_{uv} & \text{if } (u, v) \in D_L, \\ 0 & \text{otherwise,} \end{cases} \quad \text{and}$$

$$\Lambda_{uv}^R = \begin{cases} \lambda_{uv} & \text{if } (u, v) \in D_R, \\ 0 & \text{otherwise.} \end{cases}$$

Define a network  $G_{\text{flow}}^* = (V^*, D^*)$  with vertex set  $V^* = \{1, \dots, n\} \cup \{1', \dots, n'\}$ , edge set  $D^*$

containing

$$i \rightarrow j \quad \text{if } (j, i) \in D_L, \quad (3.7)$$

$$i \rightarrow i' \quad \text{for all } i \in V, \quad (3.8)$$

$$i \rightarrow j' \quad \text{if } (i, j) \in B, \quad (3.9)$$

$$i' \rightarrow j' \quad \text{if } (i, j) \in D_R, \quad \text{and} \quad (3.10)$$

with all edges and vertices having capacity 1. Let  $\Gamma = (I - \Lambda^L)^{-T} \Omega (I - \Lambda^R)^{-1}$ . Then, for any  $S, T \subset V$  with  $|S| = |T| = k$ , we have that  $|\Gamma_{S,T}| = 0$  if the max-flow from  $S$  to  $T'$  in  $G_{\text{flow}}^*$  is  $< k$ .

We may now state our more general result.

**Theorem 3.8.** *Let  $G = (V, D, B)$  be a mixed graph,  $w_0 \rightarrow v \in G$ , and suppose that the edges  $w_1 \rightarrow v, \dots, w_\ell \rightarrow v \in G$  are known to be generically (rationally) identifiable. Recalling Equation (3.10), let  $G_{\text{flow}}^*$  be  $G_{\text{flow}}$  with the edges  $w'_0 \rightarrow v', \dots, w'_\ell \rightarrow v'$  removed. Suppose there are sets  $S \subset V$  and  $T \subset V \setminus \{v, w_0\}$  such that  $|S| = |T| + 1 = k$  and*

(a)  $\text{des}(v) \cap (T \cup \{v\}) = \emptyset,$

(b) *the max-flow from  $S$  to  $T' \cup \{w'_0\}$  in  $G_{\text{flow}}$  equals  $k$ , and*

(c) *the max-flow from  $S$  to  $T' \cup \{v'\}$  in  $G_{\text{flow}}^*$  is  $< k$ .*

Then  $w_0 \rightarrow v$  is rationally identifiable by the equation

$$\lambda_{w_0 v} = \frac{|\Sigma_{S, T \cup \{v\}}| - \sum_{i=1}^{\ell} \lambda_{w_i v} |\Sigma_{S, T \cup \{w_i\}}|}{|\Sigma_{S, T \cup \{w_0\}}|}. \quad (3.11)$$

*Proof.* By assumption (b) and Corollary 3.3,  $|\Sigma_{S, T \cup \{w_0\}}|$  is generically non-zero. Therefore, equation (3.11) holds if

$$|\Sigma_{S, T \cup \{v\}}| - \sum_{i=0}^{\ell} \lambda_{w_i v} |\Sigma_{S, T \cup \{w_i\}}| = 0.$$

To show this we note that, by the multilinearity of the determinant, we have

$$|\Sigma_{S,T \cup \{v\}}| - \sum_{i=0}^{\ell} \lambda_{w_i v} |\Sigma_{S,T \cup \{w_i\}}| = \begin{vmatrix} \sigma_{s_1 t_1} & \cdots & \sigma_{s_1 t_{k-1}} & \sigma_{s_1 v} - \sum_{i=0}^{\ell} \lambda_{w_i v} \sigma_{s_1 w_i} \\ \sigma_{s_2 t_1} & \cdots & \sigma_{s_2 t_{k-1}} & \sigma_{s_2 v} - \sum_{i=0}^{\ell} \lambda_{w_i v} \sigma_{s_2 w_i} \\ \vdots & \ddots & \vdots & \vdots \\ \sigma_{s_k t_1} & \cdots & \sigma_{s_k t_{k-1}} & \sigma_{s_k v} - \sum_{i=0}^{\ell} \lambda_{w_i v} \sigma_{s_k w_i} \end{vmatrix}.$$

Write  $\Gamma$  for the matrix that appears on the right-hand side of this equation.

Consider any two indices  $i$  and  $j$  with  $1 \leq i \leq k$  and  $1 \leq j \leq k-1$ . If a trek from  $s_i$  to  $t_j$  uses one of the edges  $w_m \rightarrow v$ , for  $0 \leq m \leq \ell$ , on its right-hand side then  $t_j \in \text{des}(v)$ , a contradiction since  $\text{des}(v) \cap T = \emptyset$  by assumption (a). Similarly, since  $v \notin \text{des}(v)$  the difference  $\sigma_{s_i v} - \sum_{j=0}^{\ell} \lambda_{w_j v} \sigma_{s_i w_j}$  is obtained by summing the monomials for treks between  $s_i$  and  $v$  which do not use any edge  $w_j \rightarrow v$  on their right side. From this we may write

$$\Gamma = ((I - \Lambda)^{-T} \Omega (I - \Lambda')^{-1})_{S, T \cup \{v\}}$$

where  $\Lambda'$  equals  $\Lambda$  but with its  $(w_j, v)$ ,  $0 \leq j \leq \ell$ , entries set to 0. The fact that  $|\Gamma| = 0$  under assumption (c) is the content of Lemma 3.7 (where we take  $\Lambda^L = \Lambda$  and  $\Lambda^R = \Lambda'$ ). Given this lemma our desired result then follows.  $\square$

Clearly Theorem 3.8 can be applied whenever Theorem 3.5 can. Moreover, as the next example shows, there are cases in which Theorem 3.8 can be used while Theorem 3.5 cannot.

**Example 3.9.** Let  $G = (V, D, B)$  be the mixed graph from Figure 3.2. Take  $S = \{3, 5\}$  and  $T = \{4\}$ . Then Theorem 3.8 implies that  $\lambda_{12}$  is rationally identifiable. Theorem 3.5 cannot be applied in this case as  $S \cap \text{des}(2) \neq \emptyset$ .

For a fixed choice of  $S$  and  $T$ , the conditions (a)-(c) in Theorem 3.8 can be verified in polynomial time. Indeed, conditions (b) and (c) involve only max-flow computations that take  $O(|V|^3)$  time in general. Condition (a) can be checked by computing the descendants of  $v$ , which can be done with any  $O(|D|)$  graph traversal algorithm (e.g., depth first search, see Cormen et al. (2009)), and then computing the intersection between the descendants and  $T \cup \{v\}$  which can be done in  $O(|V| \log |V|)$  time.

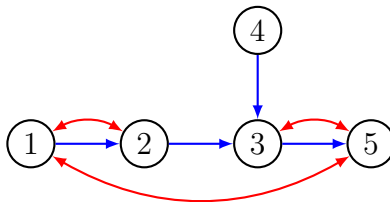


Figure 3.2: A graph for which Theorem 3.8 can be used to certify that the edge  $\lambda_{12}$  is identifiable when Theorem 3.5 cannot.

In order to apply Theorem 3.8 algorithmically, however, we have to consider all possible subsets  $S \subset V$ ,  $T \subset V \setminus \{v, w_0\}$  and check our condition for each pair. Naively done this operation takes exponential time. It remains an interesting problem for further study to determine whether or not the problem of finding suitable sets  $S$  and  $T$  is NP-hard. We note that a similar problem arises for instrumental variables/d-separation, where van der Zander et al. (2015) were able to give a polynomial time algorithm for finding suitable sets in graphs that are acyclic. Given our results so far we will maintain polynomial time guarantees simply by considering only subsets  $S, T$  of bounded size  $|S|, |T| \leq m$ .

### 3.2 Edgewise Generic Identifiability

While our results from Section 3.1 can be used together with the half-trek criterion there is notable lack of synergy between the two methods as Theorem 3.8 requires that all directed edges incoming to a node be generically identifiable before that node can be used to prove the generic identifiability of other edges. Aiming to strengthen the half-trek criterion while allowing it to better use identifications produced by Theorem 3.8, the following theorem establishes a sufficient condition for the generic identifiability of any set of incoming edges to a fixed node. While in the process of preparing this work for publication we discovered the work of Chen (2016); our following theorem can be seen as a generalization of his Theorem 1, see Remark 3.11 for a discussion of the primary difference between our theorem and that of Chen (2016).

**Theorem 3.10.** *Let  $G = (V, D, B)$  be a, non-empty, mixed graph and let  $v \in V$ . Let  $W \subset \text{pa}(v)$  and suppose there exists  $Y \subset V \setminus (\{v\} \cup \text{sib}(v))$  with  $|Y| = |W|$  such that,*

(i) *there exists a half-trek system from  $Y$  to  $W$  with no sided intersection,*

(ii) *for every trek  $\pi$  from  $y \in Y$  to  $v$  we have that either*

(a)  *$\pi$  ends with an edge of the form  $s \rightarrow v$  where either  $s \in W$  or  $s \rightarrow v$  is known to be generically (rationally) identifiable, or*

(b)  *$\pi$  begins with an edge of the form  $y \leftarrow s$  where  $s \rightarrow y$  is known to be generically (rationally) identifiable.*

*Then for each  $w \in W$  we have that  $w \rightarrow v$  is generically (rationally) identifiable.*

*Proof.* Let  $(\Lambda, \Omega)$  be the matrices of indeterminants corresponding to  $G$ , and let  $\Sigma = (I - \Lambda)^{-T} \Omega (I - \Lambda)^{-1}$  be the covariance matrix. Recall our notation  $\mathcal{T}(x, z)$  for the set of treks from  $x$  to  $z$  in  $G$ . By the trek rule (Proposition 2.6),  $\Sigma_{xz} = \sum_{\pi \in \mathcal{T}(x, z)} \pi(\Lambda, \Omega)$  is the sum of monomials for treks from  $x$  to  $z$ .

Recalling that  $|Y| = |W|$ , enumerate  $W = \{w_1, \dots, w_k\}$  and  $Y = \{y_1, \dots, y_k\}$ . Now, for  $1 \leq i \leq k$ , let  $H_i \subset D$  be the set of all edges incoming to  $y_i$  known to be generically (rationally) identifiable.

Our approach is to build a linear system of  $k$  equations in the  $k$  unknowns  $\lambda_{w_1 v}, \dots, \lambda_{w_k v}$ , having a unique solution. Consider the set  $\mathcal{T}(y_1, v)$  of all treks between  $y_1$  and  $v$ . Because of condition (ii) we have that  $y_1 \leftrightarrow v \notin G$  and all treks from  $y_1$  to  $v$  either end in a directed edge of the form  $s \rightarrow v$ , with  $s \in W$  or  $s \rightarrow v$  known to be generically identifiable, or must start in a directed edge of the form  $y_1 \leftarrow h$  for some  $h \in H_1$ . Now note that for any  $p \in \text{pa}(v)$ ,

$$\sum_{\pi \in \mathcal{T}(y_1, p)} \pi(\Lambda, \Omega) - \sum_{h \in H_1} \sum_{\pi \in \mathcal{T}(h, p)} \pi(\Lambda, \Omega) \lambda_{p y_1} = \Sigma_{y_1 p} - \sum_{h \in H_1} \Sigma_{h p} \lambda_{h y_1}$$

equals the sum of the monomials for all treks from  $y_1$  to  $p$  that do not start with a directed edge of the form  $y_1 \leftarrow h$  for  $h \in H$ . Hence we find that the sum of all monomials for treks

from  $y_1$  to  $v$  that do not start with an edge of the form  $y_1 \leftarrow h$  for  $h \in H_1$  equals

$$\sum_{p \in \text{pa}(v)} (\Sigma_{y_1 p} - \sum_{h \in H_1} \Sigma_{hp} \lambda_{hy_1}) \lambda_{pv}.$$

Now the sum over all treks between  $y_1$  and  $v$  that start with an edge of the form  $y_1 \leftarrow h$  for  $h \in H_1$  is easily seen to be the quantity  $\sum_{h \in H_1} \Sigma_{vh} \lambda_{hy_1}$ . Thus,

$$\Sigma_{y_1 v} = \sum_{p \in \text{pa}(v)} (\Sigma_{y_1 p} - \sum_{h \in H_1} \Sigma_{hp} \lambda_{hy_1}) \lambda_{pv} + \sum_{h \in H_1} \Sigma_{vh} \lambda_{hy_1}$$

Rewriting this we have

$$\begin{aligned} & \sum_{w \in W} (\Sigma_{y_1 w} - \sum_{h \in H_1} \Sigma_{hw} \lambda_{hy_1}) \lambda_{wv} \\ &= \Sigma_{y_1 v} - \sum_{p \in \text{pa}(v) \setminus W} (\Sigma_{y_1 p} - \sum_{h \in H_1} \Sigma_{hp} \lambda_{hy_1}) \lambda_{pv} - \sum_{h \in H_1} \Sigma_{vh} \lambda_{hy_1}. \end{aligned}$$

Notice that, in the above equation, if  $p \in \text{pa}(v) \setminus W$  and  $\Sigma_{y_1 p} - \sum_{h \in H_1} \Sigma_{hp} \lambda_{hy_1} \neq 0$  then it must be the case that there is a trek  $\pi$  from  $y_1$  to  $v$  ending in the edge  $p \rightarrow v$  which does not start with an edge of the form  $y_1 \leftarrow s$  where  $s \rightarrow y_1$  is known to be generically identifiable. It then follows, by condition (ii)(a), that since  $p \notin W$  we must have that  $\lambda_{pv}$  is known to be generically identifiable. It then follows that the only unknowns quantities (that is, those not assumed to be generically identifiable) in the above displayed equation are the  $\lambda_{wv}$  which appear linearly on the left hand side. Thus we have exhibited one linear equation in the  $k$  unknown parameters  $\lambda_{w_j v}$ .

Repeating the above argument for each of the  $y_i$ , we obtain  $k$  linear equations in  $k$  unknowns. It remains to show that the system of equations is generically non-singular. This amounts to showing generic invertibility for the  $k \times k$  matrix  $A$  with entries

$$A_{ij} = \Sigma_{y_i w_j} - \sum_{h \in H_i} \Sigma_{hw_j} \lambda_{hy_i}.$$

The invertibility of  $A$  follows from the existence of the half-trek system from  $Y$  to  $W$  with no sided intersection and Lemma 3.12 below. We conclude that each  $w_i \rightarrow v$  is generically (rationally) identifiable as claimed.  $\square$

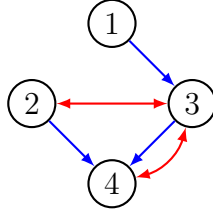


Figure 3.3: A graph that serves to illustrate differences between Theorem 1 of Chen (2016) and our Theorem 3.10.

*Remark 3.11.* Our Theorem 3.10 generalizes Theorem 1 of Chen (2016) in two ways. Firstly, we make the trivial, but for our purposes important, modification to formulate our theorem in a fashion that is agnostic as to how prior generic identifications were obtained. For the presentation in Chen (2016) it was more natural to focus only on such identifications being obtained from prior applications of his theorem. Secondly, and more substantially, the results of Chen (2016) do not consider the possibility that, recalling the setting of Theorem 3.10, some of the edges incoming to  $v$  may be known to be generically identifiable; failing to use this information makes the conditions on the set  $Y$  more restrictive. Indeed, but for our first modification, our theorem reduces to the result of Chen (2016) if we replace condition (ii)(a) by the condition “ $\pi$  ends with an edge of the form  $s \rightarrow v$  where  $s \in W$ .”

As an example of how the above difference can appear in practice consider Figure 3.3 and suppose we have restricted the size of edge sets  $W$  we consider to be of size 1 (for larger graphs, this may be required for computational efficiency). Then, using  $Y = \{1\}$  and  $W = \{3\}$ , one easily checks that  $3 \rightarrow 4$  is generically identifiable. But now, showing that  $2 \rightarrow 4$  is generically identifiable using  $W = \{2\}$  is impossible using Theorem 1 of Chen (2016) because of the trek  $2 \leftrightarrow 3 \rightarrow 4$  but this trek provides no problem for Theorem 3.10 as we have already shown that  $3 \rightarrow 4$  is generically identifiable.

The following lemma generalizes Lemma 2 from Foygel et al. (2012a) and completes the proof of Theorem 3.10.

**Lemma 3.12.** *Let  $G = (V, D, B)$  be a mixed graph on  $n$  nodes with associated covariance*

matrix  $\Sigma$ . Moreover, let  $S = \{s_1, \dots, s_k\}$ ,  $T = \{t_1, \dots, t_k\} \subset V$ . For every  $1 \leq i \leq k$  let  $H_i = \{h_1^i, \dots, h_{\ell_i}^i\} \subset \text{pa}(s_i)$ . Suppose there exists a half-trek system from  $S$  to  $T$  with no sided intersection. Then the  $k \times k$  matrix  $A$  defined by

$$A_{ij} = \Sigma_{s_i t_j} - \sum_{k=1}^{\ell_i} \Sigma_{h_k^i t_j} \lambda_{h_k^i s_i}$$

is generically invertible.

The proof of this lemma is deferred to Appendix A. Note that if let  $W = \text{pa}(v)$  and strengthen condition (ii)(b) to require that all edges incoming to  $y$  be generically identifiable whenever there exists a half-trek from  $v$  to  $y$ , then Theorem 3.10 reduces to Theorem 2.11 of Foygel et al. (2012a), the usual half-trek identifiability theorem.

The conditions of Theorem 3.10 can be easily checked in polynomial time using max-flow computations, just as with the standard half-trek criterion. Unfortunately, in general, we do not know for which subset  $W \subset \text{pa}(v)$  we should be checking the conditions of Theorem 3.10. This, in practice, means that we will have to check all subsets  $W \subset \text{pa}(v)$ . There are, of course, exponentially many such subsets in general. If we are in a setting where we may assume that all vertices have bounded in-degree, then checking all subsets requires only polynomial time. In the case that in-degrees are not bounded, we may also maintain polynomial time complexity by only considering subsets  $W$  of sufficiently large or small size. We provide pseudocode for an algorithm to iteratively identify the coefficients of a mixed graph leveraging Theorem 3.10 in Algorithm 1.

### 3.3 Edgewise Generic Nonidentifiability

In prior sections we have focused solely on sufficient conditions for demonstrating the generic identifiability of edges in a mixed graph. This, of course, begs the question of if there are any complementary necessary conditions. That is, if there exist conditions that, when failed, show that a given edge is generically many-to-one. To our knowledge, the following is the only known necessary condition for generic identifiability and considers all parameters of a mixed graph  $G$  simultaneously.

**Theorem 3.13** (Theorem 2 of Foygel et al. (2012a)). *Suppose  $G = (V, D, B)$  is a mixed graph in which every family  $(Y_v : v \in V)$  of subsets of the vertex set  $V$  either contains a set  $Y_v$  that fails to satisfy the half-trek criterion with respect to  $v$  or contains a pair of sets  $(Y_v, Y_w)$  with  $v \in Y_w$  and  $w \in Y_v$ . Then the parameterization  $\varphi_G$  is generically infinite-to-one.*

This theorem operates by showing that, given its conditions, the Jacobian of the map  $\varphi_G$  fails to have full column rank and thus must have infinite-to-one fibers. Unfortunately this theorem does not give any indication regarding which edges are, in particular, generically infinite-to-one. Our theorem below gives a simple condition which guarantees that a directed edge is generically infinite-to-one.

**Theorem 3.14.** *Let  $G = (V, D, B)$  be a mixed graph and let  $v \rightarrow w \in G$ . Suppose that for every  $z \in V \setminus \{w\}$  we have either  $z \leftrightarrow w \in G$  or  $v$  is not half-trek reachable from  $z$ . Let  $\text{proj}_{v \rightarrow w}$  be the projection  $(\Lambda, \Omega) \mapsto \lambda_{vw}$  for  $v \rightarrow w \in G$ . Then  $\text{proj}_{v \rightarrow w}(\mathcal{F}(\Lambda, \Omega))$  is infinite for all  $(\Lambda, \Omega) \in \Theta = \mathbb{R}_{\text{reg}}^D \times PD(B)$ .*

*Proof.* Let  $(\Lambda, \Omega) \in \Theta$  and  $\Sigma = \varphi_G(\Lambda, \Omega) = (I - \Lambda)^{-T} \Omega (I - \Lambda)^{-1}$ . We will show that for each matrix  $\Gamma = (\gamma_{xy}) \in \mathbb{R}_{\text{reg}}^D$  that agrees with  $\Lambda$  in all but (possibly) the  $(v, w)$  entry, we can find  $\Psi \in PD(B)$  for which  $\varphi_G(\Gamma, \Psi) = \Sigma$ . The claim then follows by noting that the choices for  $\Gamma$  allow for infinitely many values of  $\gamma_{vw}$ .

Let  $\Gamma \in \mathbb{R}_{\text{reg}}^D$  be as above, and let  $x \neq y \in V$  be such that  $x \leftrightarrow y \notin G$ . Then

$$\begin{aligned} & ((I - \Gamma)^T \Sigma (I - \Gamma))_{xy} \\ &= \sigma_{xy} - \sum_{z \in \text{pa}(x)} \sigma_{yz} \gamma_{zx} - \sum_{z \in \text{pa}(y)} \sigma_{xz} \gamma_{zy} + \sum_{z \in \text{pa}(x)} \sum_{z' \in \text{pa}(y)} \gamma_{zx} \gamma_{z'y} \sigma_{zz'}. \end{aligned}$$

Whenever  $x, y \neq w$  then  $\gamma_{zx} = \lambda_{zx}$  and  $\gamma_{zy} = \lambda_{zy}$  in the above equation. Thus

$$0 = \Omega_{xy} = ((I - \Lambda)^T \Sigma (I - \Lambda))_{xy} = ((I - \Gamma)^T \Sigma (I - \Gamma))_{xy}.$$

Next suppose, without loss of generality, that  $x = w$  and  $y \neq w$ . Then, since  $y$  is a non-sibling of  $w$ , we must have that  $v$  is not half-trek reachable from  $y$ , and hence  $\sigma_{vy} = \sum_{z \in \text{pa}(y)} \sigma_{vz} \lambda_{zy}$ .

But then

$$\begin{aligned}
& ((I - \Gamma)^T \Sigma (I - \Gamma))_{wy} \\
&= \sigma_{wy} - \sum_{z \in \text{pa}(w)} \sigma_{yz} \gamma_{zw} - \sum_{z \in \text{pa}(y)} \sigma_{wz} \gamma_{zy} + \sum_{z \in \text{pa}(w)} \sum_{z' \in \text{pa}(y)} \gamma_{zw} \gamma_{z'y} \sigma_{zz'} \\
&= -\sigma_{vy} \gamma_{vw} + \sum_{z' \in \text{pa}(y)} \gamma_{vw} \lambda_{z'y} \sigma_{vz'} \\
&\quad + \sigma_{wy} - \sum_{v \neq z \in \text{pa}(w)} \sigma_{yz} \lambda_{zw} - \sum_{z \in \text{pa}(y)} \sigma_{wz} \lambda_{zy} + \sum_{v \neq z \in \text{pa}(w)} \sum_{z' \in \text{pa}(y)} \lambda_{zw} \lambda_{z'y} \sigma_{zz'} \\
&= -\gamma_{vw} (\sigma_{vy} - \sum_{z' \in \text{pa}(y)} \lambda_{z'y} \sigma_{vz'}) \\
&\quad + \sigma_{wy} - \sum_{v \neq z \in \text{pa}(w)} \sigma_{yz} \lambda_{zw} - \sum_{z \in \text{pa}(y)} \sigma_{wz} \lambda_{zy} + \sum_{v \neq z \in \text{pa}(w)} \sum_{z' \in \text{pa}(y)} \lambda_{zw} \lambda_{z'y} \sigma_{zz'}.
\end{aligned}$$

Now since  $\sigma_{vy} - \sum_{z' \in \text{pa}(y)} \lambda_{z'y} \sigma_{vz'} = 0$ , we have that  $0 = -\gamma_{vw} (\sigma_{vy} - \sum_{z' \in \text{pa}(y)} \lambda_{z'y} \sigma_{vz'}) = -\lambda_{vw} (\sigma_{vy} - \sum_{z' \in \text{pa}(y)} \gamma_{z'y} \sigma_{vz'})$ . Therefore,

$$\begin{aligned}
& ((I - \Gamma)^T \Sigma (I - \Gamma))_{wy} \\
&= -\lambda_{vw} (\sigma_{vy} - \sum_{z' \in \text{pa}(y)} \lambda_{z'y} \sigma_{vz'}) \\
&\quad + \sigma_{wy} - \sum_{v \neq z \in \text{pa}(w)} \sigma_{yz} \lambda_{zw} - \sum_{z \in \text{pa}(y)} \sigma_{wz} \lambda_{zy} + \sum_{v \neq z \in \text{pa}(w)} \sum_{z' \in \text{pa}(y)} \lambda_{zw} \lambda_{z'y} \sigma_{zz'} \\
&= ((I - \Lambda)^T \Sigma (I - \Lambda))_{wy} \\
&= \Omega_{wy} = 0.
\end{aligned}$$

Let  $\Psi = (I - \Gamma)^T \Sigma (I - \Gamma)$ . We have just shown that  $\Psi_{xy} = 0$  for every  $x, y \in V$  such that  $x \leftrightarrow y \notin G$ . To see that  $\Psi \in PD(B)$  it remains to show that  $\Psi$  is positive definite. But this is obvious from its definition since  $\Sigma$  is positive definite and  $I - \Gamma$  is invertible. We conclude that  $\varphi_G(\Gamma, \Psi) = \Sigma$  which proves the claim.  $\square$

**Example 3.15.** Let  $G$  be the graph in Figure 3.4a. Using the necessary condition of the half-trek criterion, Theorem 3.13, we find that  $\varphi_G$  is generically infinite-to-one. To identify which



(a) A graph in which all directed edges are identifiable except  $2 \rightarrow 3$ . The  $2 \rightarrow 3$  edge can be shown to be infinite-to-one using Theorem 3.14

(b) A graph known to have generically infinite-to-one parameterization by Theorem 3.13 but for which Theorem 3.14 applies to no edge.

Figure 3.4: Examples of Theorem 3.13 and Theorem 3.14.

edges of  $G$  are themselves infinite-to-one we use Theorem 3.14. Doing so, one easily finds that the  $2 \rightarrow 3$  edge of  $G$  is generically infinite-to-one. Indeed, using the edgewise identification techniques of Section 3.2, we see that all other directed edges of  $G$  are generically identifiable so we have completely characterized which directed edges of  $G$  are, and are not, generically identifiable.

We stress, however, that Theorem 3.14 does not imply Theorem 3.13; that is, there are graphs  $G$  for which Theorem 3.13 shows  $\varphi_G$  is infinite-to-one but Theorem 3.14 cannot verify that any edges of  $G$  are infinite-to-one. For example, see Figure 3.4b.

### 3.4 Computational Experiments

In this section we will provide some computational experiments that demonstrate the usefulness of our theorems in extending the applicability of the half-trek criterion. All of our following experiments are carried out in the R programming language and the following algorithms are implemented in our R package SEMID which is available on CRAN, the Comprehensive R Archive Network (R Core Team, 2018; Foygel Barber et al., 2017), as well

as on GitHub.<sup>1</sup> We will be considering four algorithms for checking generic identifiability:

- (i) The standard half-trek criterion (HTC) algorithm.
- (ii) The edgewise identification (EID) algorithm, displayed in Algorithm 1, where the input set of *solvedEdges* is empty.
- (iii) The trek-separation identification (TSID) algorithm. Similarly as for Algorithm 1 this algorithm iteratively applies Theorem 3.8 until it fails to identify any additional edges. (Since we are considering a small number of nodes there is no need to limit the size of sets  $S$  and  $T$  we are searching for in our computation.)
- (iv) The EID+TSID algorithm. This algorithm alternates between the EID and TSID algorithms until it fails to identify any additional edges.

We emphasize that when all of the directed edges, i.e., the matrix  $\Lambda$  is generically (rationally) identifiable then we also have that  $\Omega = (I - \Lambda)^T \Sigma (I - \Lambda)$  is generically (rationally) identifiable.

In Table 1 of Foygel et al. (2012b), the authors list all 112 acyclic non-isomorphic mixed graphs on 5 nodes which are generically identifiable but for which the half-trek criterion remains inconclusive even when using decomposition techniques. We run the EID, TSID, and EID+TSID algorithms upon the 112 inconclusive graphs and find that 23 can be declared generically identifiable by the EID algorithm, 0 by the TSID algorithm, and 98 by the EID+TSID algorithm. Thus it is only by using both the determinantal equations discovered by t-separation and the edgewise identification techniques that one sees a substantial increase in the number of graphs that can be declared generically identifiable.

We observe a similar trend to the above when allowing cyclic mixed graphs. In Table 2 of Foygel et al. (2012b), the authors list 75 randomly chosen, cyclic (i.e., containing a loop in the directed part), mixed graphs that are known to be rationally identifiable but cannot

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<sup>1</sup>See <https://github.com/LucaWeihs/SEMID>.

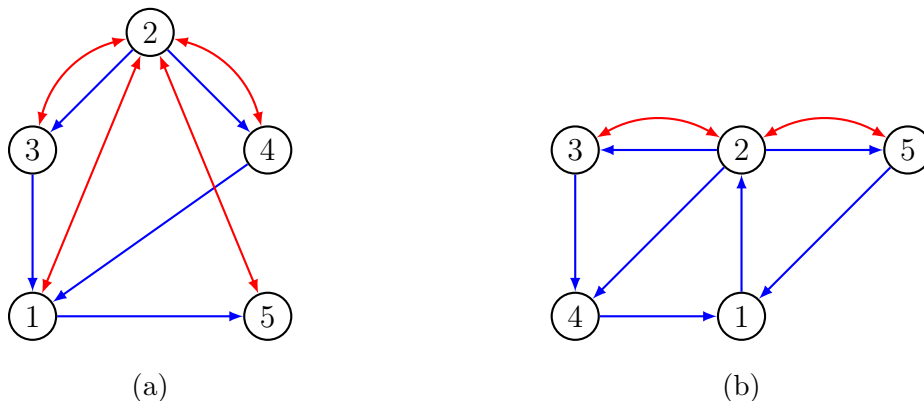


Figure 3.5: Two graphs for which the EID+TSID algorithm is inconclusive. (a) is acyclic while (b) contains a cycle.

be certified so by the half-trek criterion. Of these 75 graphs, 4 are certified to be generically identifiable by the EID algorithm, 0 by the TSID algorithm, and 34 by the EID+TSID algorithm.

A listing of the 14 acyclic and 41 cyclic mixed graphs that could not be identified by the EID+TSID algorithm are listed as integer pairs  $(d, b) \in \mathbb{N}^2$  in Table 3.1. The algorithm to convert a pair  $(d, b)$  in that table to a mixed graph  $G$  on  $n$  nodes is

1. For  $v \leftarrow 1, \dots, n$ , for  $w \leftarrow 1, \dots, v - 1, v + 1, \dots, n$ , do
  - Add edge  $v \rightarrow w$  to  $G$  if  $d \bmod 2 = 1$
  - Replace  $d$  with  $\lfloor d/2 \rfloor$
2. For  $v \leftarrow 1, \dots, n - 1$ , for  $w \leftarrow v + 1, \dots, n$ , do
  - Add edge  $v \leftrightarrow w$  to  $G$  if  $b \bmod 2 = 1$
  - Replace  $b$  with  $\lfloor b/2 \rfloor$

See Figure 3.5 for an example of a cyclic and acyclic graph that the EID+TSID algorithm fails to correctly certify as generically identifiable.

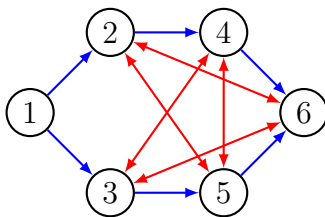


Figure 3.6: A graph where the edges  $4 \rightarrow 6$  and  $5 \rightarrow 6$  can be simultaneously proven to be generically identifiable by solving a  $2 \times 2$  linear system of determinantal equations.

### 3.5 Conclusion

By exploiting the trek-separation characterization of the vanishing of subdeterminants of the covariance matrix  $\Sigma$  corresponding to a mixed graph  $G$ , we have shown that individual edge coefficients can be generically identified by quotients of subdeterminants. This constitutes a generalization of instrumental variable techniques that are derived from conditional independence. We have also shown how this information, in concert with a generalized half-trek criterion, allows us to prove that substantially more graphs have all or some subset of their parameters generically identifiable.

Our work on identification by ratios of determinants focuses on a single edge coefficient. However, it seems possible to give a generalization that is in the spirit of the generalized instrumental sets of Brito and Pearl (2002); see also van der Zander and Liškiewicz (2016). These leverage several conditional independencies to find a linear equation system that can be used to identify several edge coefficients simultaneously, under specific assumptions on the interplay of the conditional independencies and the edges to be identified. We illustrate the idea of how to do this using general determinants in the following example. However, a full exploration of this idea is beyond the scope of this paper. In particular, we are still lacking mathematical tools that, in suitable generality, could be used to certify that constructed linear equation systems have a unique solution.

**Example 3.16.** Let  $G$  be the graph in Figure 3.6 with corresponding covariance matrix

$\Sigma = (I - \Lambda)^{-T} \Omega (I - \Lambda)^{-1}$ . Then, by similar considerations to those in Example 3.4, one may show that

$$\begin{pmatrix} |\Sigma_{\{3,5\},\{1,4\}}| & |\Sigma_{\{3,5\},\{1,5\}}| \\ |\Sigma_{\{2,4\},\{1,4\}}| & |\Sigma_{\{2,4\},\{1,5\}}| \end{pmatrix} \begin{pmatrix} \lambda_{46} \\ \lambda_{56} \end{pmatrix} = \begin{pmatrix} |\Sigma_{\{3,5\},\{1,6\}}| \\ |\Sigma_{\{2,4\},\{1,6\}}| \end{pmatrix}.$$

Using computer algebra we find that the  $2 \times 2$  matrix on the left hand side of the above equation has all non-zero polynomial entries, so that this is not equivalent to simply applying Theorem 3.8 for  $4 \rightarrow 6$  and  $5 \rightarrow 6$  separately, and has non-zero determinant. It follows that the above system is generically invertible and thus  $\lambda_{46}$  and  $\lambda_{56}$  are generically identifiable.

### ***Acknowledgments***

This material is based on work started in June 2016 at the Mathematics Research Communities (Week on Algebraic Statistics). The work was supported by the National Science Foundation under Grant Number DMS 1321794 and 1712535.

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**Algorithm 1** Edgewise identification algorithm.

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- 1: **Input:** A mixed graph  $G = (V, D, B)$  with  $V = \{1, \dots, n\}$  and a set of edges,  $solvedEdges$ , known to be generically identifiable.
  - 2: **repeat**
  - 3:   **for**  $v \leftarrow 1, \dots, n$  **do**
  - 4:      $unsolved \leftarrow \{w \in V \mid w \rightarrow v \in G \text{ and } w \rightarrow v \notin solvedEdges\}$ .
  - 5:      $maybeAllowed \leftarrow$   
        $\{y \in V \setminus (\{v\} \cup sib(v)) \mid z \in htr(v) \cap pa(y) \implies z \rightarrow y \in solvedEdges\}$
  - 6:     **for**  $\emptyset \neq W \subset unsolved$  **do**
  - 7:        $allowed \leftarrow \{y \in maybeAllowed \mid htr(y) \cap tr(\{p \in pa(y) \mid p \rightarrow y \notin solvedEdges\}) \cap unsolved \subset W\}$
  - 8:        $exists \leftarrow$  Using max-flow computations, does there exist a half-trek system from  $allowed$  to  $W$  of size  $|W|$  with no sided intersection?
  - 9:       **if**  $exists$  is true **then**
  - 10:           $solvedEdges \leftarrow solvedEdges \cup \{e \rightarrow v \mid e \in E\}$
  - 11:          Break out of the current loop
  - 12:       **end if**
  - 13:     **end for**
  - 14: **end for**
  - 15: **until** No additional edges have been added to  $solvedEdges$  on the most recent loop.
  - 16: **Output:**  $solvedEdges$ , the set of edges found to be generically (rationally) identifiable.
-

Acyclic	Cyclic		
(4456, 113)	(345, 440)	(6629, 512)	(75321, 516)
(360, 117)	(71329, 18)	(74536, 788)	(75398, 20)
(6275, 172)	(81089, 0)	(5545, 96)	(70803, 896)
(6307, 172)	(4714, 41)	(75112, 72)	(4457, 592)
(6275, 188)	(70881, 80)	(74970, 4)	(74883, 522)
(360, 369)	(74963, 512)	(4579, 384)	(350, 112)
(4696, 401)	(74886, 268)	(70594, 65)	(74883, 2)
(4936, 401)	(5058, 304)	(74921, 66)	(74950, 260)
(4936, 402)	(70821, 513)	(70474, 640)	(74890, 38)
(4680, 403)	(74915, 6)	(74922, 66)	(81076, 0)
(840, 466)	(5267, 82)	(13160, 65)	(70851, 32)
(5257, 658)	(76852, 128)	(4938, 448)	(1430, 120)
(5257, 659)	(71075, 516)	(4730, 640)	(5251, 418)
(4680, 914)	(4397, 897)	(70358, 1)	

Table 3.1: *Of the 112 acyclic and 75 cyclic mixed graphs on 5 nodes described in Tables 1 and 2 of Foygel et al. (2012b), we display the 12 acyclic and 41 cyclic graphs which are known to be generically identifiable but for which the EID+TSID algorithm could not certify that all edges were generically identifiable. Each graph is encoded as a pair  $(d, b)$ , see text for details.*

## Appendix A

### PROOFS FOR PART I

#### PROOF OF LEMMA 3.7

We will require a known generalization of the Gessel-Viennot-Lindström lemma which we now state.

**Definition A.1.** Let  $G = (V, D)$  be a directed graph with vertices  $V = \{1, \dots, n\}$  and corresponding matrix of indeterminants  $\Lambda$ . Let  $\pi = v_1 \rightarrow v_2 \rightarrow \dots \rightarrow v_\ell$  be a directed path in  $G$ . Then define the *loop erased* path  $LE(\pi)$  corresponding to  $\pi$  recursively as follows. If  $\pi$  contains no loops then  $\pi = LE(\pi)$ . Otherwise there exist indices  $1 \leq i < j \leq \ell$  such that  $v_i = v_j$ . Then  $LE(\pi) = LE(\pi')$  where  $\pi' = v_1 \rightarrow v_2 \rightarrow \dots \rightarrow v_i \rightarrow v_{j+1} \rightarrow \dots \rightarrow v_\ell$ . It can be shown that  $LE(\pi)$  is well defined (i.e. is independent of the ordering of the above recursion).

**Lemma A.2** (Gessel-Viennot-Lindström Generalization, Theorem 6.1 of Fomin (2001)).  
*Let  $G = (V, D)$  be a directed graph with vertices  $V = \{1, \dots, n\}$  and corresponding matrix of indeterminants  $\Lambda$ . Define  $\Psi = (I - \Lambda)^{-1}$  and for any directed path  $\pi$  in  $G$  define the path polynomial  $\pi(\Lambda) = \prod_{w \rightarrow v \in \pi} \lambda_{wv}$ . Then for any  $S = \{s_1, \dots, s_k\}, T = \{t_1, \dots, t_k\} \subset V$  we have that*

$$|\Psi_{S,T}| = \sum_{\tau \in P_n} \text{sign}(\tau) \sum_{\substack{s_1 \xrightarrow{\pi_1} t_{\tau(1)}, \dots, s_k \xrightarrow{\pi_k} t_{\tau(k)} \\ i < j \implies \pi_j \cap LE(\pi_i) = \emptyset}} \pi_1(\Lambda) \dots \pi_k(\Lambda),$$

here the above inner sum is over all directed path systems  $\Pi = \{\pi_1, \dots, \pi_k\}$  with  $\pi_i$  going from  $s_i$  to  $t_{\tau(i)}$  for all  $i$ , where  $\pi_j$  and  $LE(\pi_i)$  share no vertices for  $i < j$ . Hence  $|\Psi_{S,T}| = 0$  if and only if every system of directed paths from  $S$  to  $T$  has two paths which share a vertex.

The remaining proof of Lemma 3.7 proceeds in several parts and closely follows similar results in Sullivant et al. (2010) and Draisma et al. (2013). As such we will state several lemmas whose proofs require only small modifications of existing results (such as replacing the standard Gessel-Viennot-Lindström Lemma with its generalization above). In such cases we will simply direct the reader to the corresponding proof and sketch the necessary modifications.

**Definition A.3.** Let  $G = (V, D, B)$  be a mixed graph and let  $U \subset D$ . We say a trek  $\pi$  in  $G$  *avoids  $U$  on the left (right)* if the left (right) side of  $\pi$  uses no edges from  $U$ . Similarly we say a system of treks  $\Pi$  in  $G$  *avoids  $U$  on the left (right)* if every trek  $\pi \in \Pi$  avoids  $U$  on the left (right). If  $U_L, U_R \subset D$  we say that a *trek (or trek system) avoids  $(U_L, U_R)$*  if it avoids  $U_L$  on the left and  $U_R$  on the right.

**Lemma A.4.** Let  $G = (V, D, B)$  be a mixed graph and let  $\Lambda, \Omega$  be  $n \times n$  matrices of indeterminants corresponding to the directed and bidirected parts of  $G$  respectively. Suppose that  $B = \emptyset$  so that  $\Omega$  is diagonal. Letting  $D_L, D_R, \Lambda^L, \Lambda^R, \Gamma$ , and  $G_{\text{flow}}^*$  be as in Lemma 3.7 we have that for any  $S, T \subset V$  with  $|S| = |T| = k$ ,  $|\Gamma_{S,T}| = 0$  if and only if the max-flow from  $S$  to  $T'$  in  $G_{\text{flow}}^*$  is  $< k$ .

*Proof.* In the following, whenever we say “As in x,” we mean “As in the proof of x in Sullivant et al. (2010).”

As in Lemma 3.2, we have  $|\Gamma_{S,T}| = 0$  if and only if for every set  $A \subset V$  with  $|A| = K$  we have  $|((I - \Lambda^L)^{-1})_{S,A}| = 0$  or  $|((I - \Lambda^R)^{-1})_{A,T}| = 0$ . As in Prop. 3.5, using the above result, and applying our version of the Gessel-Viennot-Lindström Lemma, we have that  $|\Gamma_{S,T}| = 0$  if and only if every system of (simple) treks avoiding  $(D \setminus D_L, D \setminus D_R)$  has sided intersection.

Now noticing that  $B = \emptyset$  simplifies the definition of  $G_{\text{flow}}^*$ , we have as in Prop. 3.5 that the (simple) treks from  $u$  to  $v$  avoiding  $(D \setminus D_L, D \setminus D_R)$  in  $G$  are in bijective correspondence with directed paths from  $u$  to  $v'$  in  $G_{\text{flow}}^*$ . Finally the result follows by noticing that max-flow systems from  $S$  to  $T'$  in  $G_{\text{flow}}^*$  of size  $k$  correspond to systems of treks from  $S$  to  $T$

avoiding  $(D \setminus D_L, D \setminus D_R)$  with no-sided intersection (that is, if one exists so does the other). Combining the above if and only if statements, the result then follows.  $\square$

We have now proven our desired result in the case  $B = \emptyset$ , it remains to show that this implies the case  $B \neq \emptyset$ . To this end, we say that  $\tilde{G} = (\tilde{V}, \tilde{D}, \tilde{B})$  is the *bidirected subdivision* of  $G = (V, D, B)$  if it equals  $G$  but where we have replaced every bidirected edge  $i \leftrightarrow j \in G$  with a vertex  $v_{(i,j)}$  and two edges  $v_{(i,j)} \rightarrow i$  and  $v_{(i,j)} \rightarrow j$  (with associated parameters  $\tilde{\omega}_{(i,j),(i,j)}, \tilde{\lambda}_{(i,j)i}, \tilde{\lambda}_{(i,j)j}$ ). Note that we have subdivided every bidirected edge into two directed edges which motivates the naming convention. Let  $\tilde{D}_L$  and  $\tilde{D}_R$  be equal to  $D_L$  and  $D_R$  respectively but where we have also added in the new edges  $v_{(i,j)} \rightarrow i$  and  $v_{(i,j)} \rightarrow j$  for every  $i \leftrightarrow j \in G$ . Let  $\tilde{\Lambda}, \tilde{\Omega}$  be matrices of indeterminants corresponding to  $\tilde{G}$  and let  $\tilde{\Lambda}^L, \tilde{\Lambda}^R$  correspond to  $\tilde{D}_L, \tilde{D}_R$  just as for  $G$ . We now have the following result that relates  $G$  and  $\tilde{G}$ .

**Lemma A.5.** *Let  $G, \tilde{G}$  be as in the prior paragraph. Then letting  $\tilde{\Gamma} = (I - \tilde{\Lambda}^L)^{-T} \tilde{\Omega} (I - \tilde{\Lambda}^R)^{-1}$  we have that, for any polynomial  $f$  taking, as input, an  $n \times n$  matrix of variables, we have that  $f(\Gamma) = 0$  if and only if  $f(\tilde{\Gamma}) = 0$ . In particular, since the subdeterminant of a matrix is a polynomial in the entries of the matrix, we have that for any  $S, T \subset V$  with  $|S| = |T| = k$ ,  $|\Gamma_{S,T}| = 0$  if and only if  $|\tilde{\Gamma}_{S,T}| = 0$ .*

*Proof.* This proof follows, essentially exactly, as the first part of the proof of Prop. 2.5 in Draisma et al. (2013).  $\square$

Now we show that the above subdivision trick produces a graph  $\tilde{G}_{\text{flow}}^*$  for which the max-flow between vertex sets is the same as for  $G_{\text{flow}}^*$ .

**Lemma A.6.** *Consider the graphs  $G_{\text{flow}}^* = (V^*, D^*)$  from the Lemma 3.7 statement and let  $\tilde{G}_{\text{flow}}^* = (\tilde{V}^*, \tilde{D}^*)$  be corresponding flow graph for the bidirected subdivision  $\tilde{G}$  of  $G$ . Let  $S = \{s_1, \dots, s_k\}$ ,  $T = \{t_1, \dots, t_k\} \subset V$ . Then the maximum flow from  $S$  to  $T' = \{t'_1, \dots, t'_k\}$  in  $G_{\text{flow}}^*$  equals the maximum flow from  $S$  to  $T'$  in  $\tilde{G}_{\text{flow}}^*$ .*

*Proof.* Recall that a flow system on a graph is an assignment of flow to the edges and vertices of the graph satisfying the usual flow constraints. Also recall that, for graphs with integral

capacities, there always exists a max-flow system between subsets of nodes for which all flow assignments upon edges and vertices take values in  $\mathbb{N}$ . We will show that any (integral valued) max-flow system from  $S$  to  $T'$  in  $\tilde{G}_{\text{flow}}^*$  corresponds to a unique flow system in  $G_{\text{flow}}^*$  with the same total flow and vice-versa. Our result then follows.

Let  $\tilde{\mathcal{F}}$  be a max-flow system from  $S$  to  $T'$  on  $\tilde{G}_{\text{flow}}^*$  from  $S$  to  $T'$  with integral flow assignments. Since  $\tilde{G}_{\text{flow}}^*$  and  $G_{\text{flow}}^*$  have all capacities equal to 1 it follows that  $\tilde{\mathcal{F}}$  assigns either 0 or 1 flow to all edges and vertices in the graph.

We now construct a flow system  $\mathcal{F}$  on  $G_{\text{flow}}^*$  with the same capacity. First let  $\mathcal{F}$  assign the same capacity to all edges and vertices that  $\mathcal{F}$  shares with  $\tilde{\mathcal{F}}$ . Note that if  $\tilde{\mathcal{F}}$  does not assign any flow to any of the edges incoming to the vertices  $v_{(i,j)}$  then  $\mathcal{F}$  already corresponds to a flow system on  $G_{\text{flow}}^*$  with the same total flow. Suppose otherwise that  $\tilde{\mathcal{F}}$  assigns 1 unit of flow to the edges  $\{a_1 \rightarrow v_{a_1 b'_1}, \dots, a_k \rightarrow v_{a_k b'_k}\}$ . Since  $v_{(i,j)}$  and the  $a_i$  have capacity 1 it follows that  $a_i \neq a_j$  and  $v_{a_i b'_i} \neq v_{a_j b'_j}$  for all  $i \neq j$ . For each edge  $a_i \rightarrow v_{a_i b'_i}$ , since  $v_{a_i b'_i}$  has two outgoing edges  $v_{a_i b'_i} \rightarrow a'_i$  and  $v_{a_i b'_i} \rightarrow b'_i$ , there are two possible cases:

- Case 1:  $\tilde{\mathcal{F}}$  assigns 1 flow to  $v_{a_i b'_i} \rightarrow a'_i$ .

In this case assign a flow of 1 to the edge  $a_i \rightarrow a'_i$  in  $\mathcal{F}$ .

- Case 2:  $\tilde{\mathcal{F}}$  assigns 1 flow to  $v_{a_i b'_i} \rightarrow b'_i$ .

In this case assign a flow of 1 to the edge  $a_i \rightarrow b'_i$  in  $\mathcal{F}$ .

It is easy to check that  $\mathcal{F}$  is indeed a valid flow system on  $G_{\text{flow}}^*$  with the same flow as  $\tilde{\mathcal{F}}$ .

To see the opposite direction let  $\mathcal{F}$  be a max-flow system from  $S$  to  $T'$  on  $G_{\text{flow}}^*$  from  $S$  to  $T'$  with integral flow assignments. We now construct a flow system  $\tilde{\mathcal{F}}$  on  $\tilde{G}_{\text{flow}}^*$  with the same capacity. As before, first let  $\tilde{\mathcal{F}}$  assign the same capacity to all edges and vertices that  $\tilde{\mathcal{F}}$  shares with  $\mathcal{F}$ . Note that if  $\mathcal{F}$  does not assign any flow to any of the edges  $a \rightarrow b'$  for  $(a, b) \in B$  then  $\tilde{\mathcal{F}}$  already corresponds to a flow system on  $G_{\text{flow}}^*$  with the same total flow. Suppose otherwise that  $\tilde{\mathcal{F}}$  assigns 1 unit of flow to the edges  $E = \{a_1 \rightarrow b'_1, \dots, a_k \rightarrow b'_k\}$

with  $(a_i, b_i) \in B$  for all  $i$ . Since all vertices in  $\mathcal{F}$  have capacity 1 we must have that  $a_i \neq a_j$  and  $b_i \neq b_j$  for all  $i \neq j$ . There are two possible cases:

- Case 1:  $a_i \rightarrow b'_i \in E$  and  $b_i \rightarrow a_i \notin E$ .

In this case assign a flow of 1 along the path  $a_i \rightarrow v_{a_i b_i} \rightarrow b'_i$  in  $\tilde{\mathcal{F}}$ .

- Case 2:  $a_i \rightarrow b'_i \in E$  and  $b_i \rightarrow a_i \in E$ .

In this case assign a flow of 1 to the edges  $a_i \rightarrow a'_i$  and  $b_i \rightarrow b'_i$  in  $\tilde{\mathcal{F}}$ .

One may now check that  $\tilde{\mathcal{F}}$  is a valid flow system on  $\tilde{G}_{\text{flow}}^*$  with the same flow as  $\mathcal{F}$ .  $\square$

Finally we are in a position to easily prove Lemma 3.7. Note that, by Lemma A.5 we have that  $|\Gamma_{S,T}| = 0$  if and only if  $|\tilde{\Gamma}_{S,T}| = 0$ . By Lemma A.4 we have that  $|\tilde{\Gamma}_{S,T}| = 0$  if and only if the max-flow from  $S$  to  $T'$  in  $\tilde{G}_{\text{flow}}^*$  equals  $|S| = k$ . Finally Lemma A.6 gives us that the max-flow from  $S$  to  $T'$  in  $\tilde{G}_{\text{flow}}^*$  equals the max-flow from  $S$  to  $T'$  in  $G_{\text{flow}}^*$ . Hence we have that  $|\Gamma_{S,T}| = 0$  if and only if the max-flow from  $S$  to  $T'$  in  $G_{\text{flow}}^*$  equals  $k$ , this was our desired statement.  $\square$

### PROOF OF LEMMA 3.12

The proof of this lemma follows almost identically as the proof of Lemma 2 in Foygel et al. (2012a). We simply restate the arguments there in our setting. For any  $v, w \in V$  let  $\mathcal{H}(v, w)$  be the set of half treks from  $v$  to  $w$  in  $G$ . Also let  $\mathcal{T}_{ij}$  be the set of all treks from  $s_i$  to  $t_j$  in  $G$  which do not begin with an edge of the form  $s_i \leftarrow h_k^i$  for any  $1 \leq k \leq \ell_i$ . Then it is easy to see that  $\mathcal{H}(s_i, t_j) \subset \mathcal{T}_{ij}$ . Now, by the trek rule (Proposition 2.6), we have that

$$A_{ij} = \sum_{\pi \in \mathcal{T}_{ij}} \pi(\Lambda, \Omega).$$

Now for any system of treks  $\Pi$  define the monomial

$$\Pi(\Lambda, \Omega) = \prod_{\pi \in \Pi} \pi(\Lambda, \Omega).$$

Then, by Leibniz's formula for the determinant, we have that

$$|A| = \sum_{\Pi} (-1)^{\text{sign}(\Pi)} \Pi(\Lambda, \Omega) \quad (\text{A.1})$$

where the above sum is over all trek systems  $\Pi$  from  $S$  to  $T$  using treks only in the set  $\cup_{1 \leq i, j \leq k} \mathcal{T}_{ij}$ ; here the  $\text{sign}(\Pi)$  is the sign of the permutation that writes  $t_1, \dots, t_k$  in the order of their appearance as targets of the treks in  $\Pi$ .

By assumption, there exists a half-trek system from  $S$  to  $T$  with no-sided intersection. Since such a system exists, let  $\Pi$  be a half-trek system of minimum total length among all such half-trek systems. Since  $\mathcal{H}(s_i, t_j) \subset \mathcal{T}_{ij}$  for all  $i, j$  it follows that  $\Pi$  is included as one of the trek systems in the summation (A.1). Let  $\Psi$  be any system of treks from  $S$  to  $T$  such that  $\Psi(\Lambda, \Omega) = \Pi(\Lambda, \Omega)$ . Lemma 1 of Foygel et al. (2012a) proves that we must have  $\Psi = \Pi$  so that  $\Pi$  is the unique system of treks from  $S$  to  $T$  with corresponding trek monomial  $\Pi(\Lambda, \Omega)$ . It thus follows that the coefficient of the monomial  $\Pi(\Lambda, \Omega)$  in  $|A|$  is  $(-1)^{\text{sign}(\Pi)}$  and thus  $|A|$  is not the zero polynomial (or power series if the sum is infinite). Hence, for generic choices of  $(\Lambda, \Omega)$ , we have that  $|A| \neq 0$  so that  $A$  is generically invertible.  $\square$

## Part II

**RANK STATISTICS FOR MEASURING DEPENDENCE**

## Chapter 4

## INTRODUCTION AND PRELIMINARIES

Many applications require a quantification of the dependence between collections of random variables. Letting  $X = (X_1, \dots, X_r)$  and  $Y = (Y_1, \dots, Y_s)$  be random vectors, we are interested in measures of dependence  $\mu$  which exhibit the following three properties:

*Property 4.1* (I-consistency). If  $X, Y$  are independent then  $\mu(X, Y) = 0$ .

*Property 4.2* (D-consistency). If  $X, Y$  are dependent then  $\mu(X, Y) \neq 0$ .

*Property 4.3* (Monotonic invariance). If  $f_1, \dots, f_r, g_1, \dots, g_s$  are strictly increasing functions then  $\mu(X, Y) = \mu\{(f_1(X_1), \dots, f_r(X_r)), (g_1(Y_1), \dots, g_s(Y_s))\}$ . We also refer to this property as  $\mu$  being *nonparametric*.

If  $\mu$  is I-consistent then tests of independence can be based on the null hypothesis  $\mu(X, Y) = 0$ . If  $\mu$  is also D-consistent then tests based on consistent estimators of  $\mu$  are guaranteed to asymptotically reject independence when it fails to hold. When  $\mu$  is both I- and D-consistent we will simply call it *consistent*. Monotonic invariance is the intuitive requirement that the level of dependence between two random vectors is invariant to monotonic transformations of any coordinate. Unfortunately, many popular measures of dependence fail to satisfy all of these properties. For instance, Kendall's  $\tau$  (Kendall, 1938) and Spearman's  $\rho$  (Spearman, 1904) are nonparametric and I-consistent but not D-consistent, while the distance correlation (Székely et al., 2007) is consistent but not nonparametric.

For bivariate observations, Hoeffding (1948) introduced a nonparametric dependence measure that is consistent for a large class of continuous distributions. Let  $(X, Y)$  be a random vector taking values in  $\mathbb{R}^2$ , with joint and marginal distribution functions  $F_{XY}, F_X,$

and  $F_Y$ . Then the statistic now called Hoeffding's  $D$ , is defined as

$$D := \int_{\mathbb{R}^2} \{F_{XY}(x, y) - F_X(x)F_Y(y)\}^2 dF_{XY}(x, y).$$

Bergsma and Dassios (2014) introduced a new bivariate dependence measure  $\tau^*$  that is nonparametric and improves upon Hoeffding's  $D$  by guaranteeing consistency for all bivariate mixtures of continuous and discrete distributions. As its name suggests,  $\tau^*$  generalises Kendall's  $\tau$ ; where  $\tau$  counts concordant and discordant pairs of points,  $\tau^*$  counts concordant and discordant quadruples of points. The proof of consistency of  $\tau^*$  is considerably more involved than that for  $D$ .

Both  $D$  and  $\tau^*$  exhibit symmetries that are obfuscated by their usual definitions. Indeed, as will be made precise,  $D$  and  $\tau^*$  can be represented as the covariance between signed sums of indicator functions acted on by the subgroup  $H = \langle (1\ 4), (2\ 3) \rangle$  of the symmetric group on four elements. In Chapter 5 we generalise this observation to define a new class of dependence measures called *symmetric rank covariances*. All such measures are I-consistent, nonparametric, and include  $D$ ,  $\tau^*$ ,  $\tau$ , and  $\rho$  as special cases. Moreover, our new measures include natural multivariate extensions of  $\tau^*$  which themselves inspire new notions of concordance and discordance in higher dimensions; see Figure 4.1. While symmetric rank covariances need not be D-consistent, we identify a sub-collection of measures that are. These consistent measures can be interpreted as testing independence by applying possibly infinitely many independence tests to discretizations of  $(X, Y)$ . In Chapter 6 we show that symmetric rank covariances can readily be estimated using U-statistics and, through the use of efficient data structures for orthogonal range queries, find that many of these U-statistics can be computed efficiently. Chapter 7 then considers the large-sample behavior of the above U-statistics; in particular we show that, under the null hypothesis of independence and certain general conditions, these U-statistics are degenerate of order two, thus having non-Gaussian limiting distributions. Moreover, in the bivariate setting, we explicitly describe the limiting distribution for the U-statistic estimating  $\tau^*$  and show that, under some weak distributional assumptions, it is a scale multiple of the asymptotic

distribution for the U-statistic estimating  $D$ .

While our work can be seen as an extension and generalisation of classical rank statistics for measuring association, recent interest in dependence testing has produced a variety of approaches to the problem. Broadly these alternative measures can be organized into those that are based on information theory (Kraskov et al., 2004; Kinney and Atwal, 2014; Reshef et al., 2011, 2015), characteristic functions (Kankainen and Ushakov, 1998; Meintanis, 2008; Székely et al., 2007; Rizzo and Szekely, 2016; Böttcher et al., 2017), grid/binning procedures (Heller et al., 2013, 2016; ?), reproducing kernel Hilbert spaces (Gretton et al., 2005), conditional distribution functions (Cui et al., 2015), and generalising or modifying Pearson’s correlation coefficient (Breiman and Friedman, 1985; Zhu et al., 2017; Wang et al., 2017). While each of these measures has distinct advantages, our experiments show that symmetric rank covariances are competitive in a number of regimes while remaining simple to state and interpret.

In the remainder of this chapter we will introduce the basic group theory necessary to define symmetric rank covariances and give formal introductions to the  $D$  and  $\tau^*$  measures which our work generalises.

#### 4.1 *Permuting Vectors via a Group Action*

We begin by establishing conventions and notation used throughout the paper. Let

$$(Z_1, \dots, Z_{r+s}) = Z = (X, Y) = (X_1, \dots, X_r, Y_1, \dots, Y_s)$$

be a random vector taking values in  $\mathbb{R}^{r+s}$ , and let  $(X^i, Y^i) = Z^i$  for  $i \in \mathbb{Z}_{>0}$  be a sequence of independent and identically distributed copies of  $Z$ . When  $X$  and  $Y$  are independent we write  $X \perp\!\!\!\perp Y$ , otherwise we write  $X \not\perp\!\!\!\perp Y$ . We let  $F_{XY}, F_X$ , and  $F_Y$  denote the cumulative distribution functions for  $(X, Y)$ ,  $X$ , and  $Y$ , respectively.

We will require succinct notation to describe tuples of vectors, possibly permuted. For any  $n \geq 1$ , define  $[n] := \{1, \dots, n\}$ . Let  $w^1, \dots, w^n \in \mathbb{R}^d$ . Then for  $i_1, \dots, i_m, j_1, \dots, j_k \in [n]$ ,

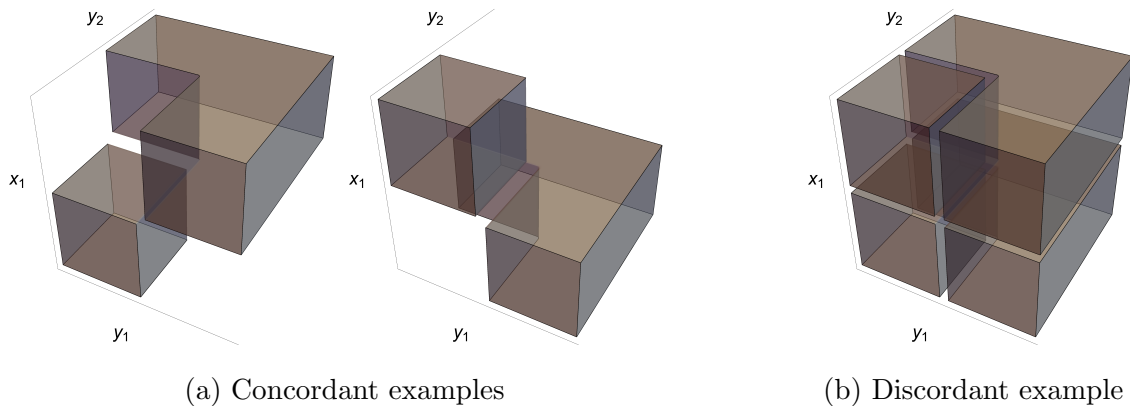


Figure 4.1: The bivariate sign covariance  $\tau^*$  can be defined in terms of the probability of concordance and discordance of four points in  $\mathbb{R}^2$  (Bergsma and Dassios, 2014, Figure 3). Our multivariate extension  $\tau_P^*$  is based on higher-dimensional generalisations of concordance and discordance. For illustration, let  $x^1, \dots, x^4 \in \mathbb{R}$  and  $y^1, \dots, y^4 \in \mathbb{R}^2$ . Considering either plot in panel (a), if precisely two tuples  $(x^i, y^i)$  fall in each of the two gray regions, then the four tuples are concordant for  $\tau_P^*$ , but other types of concordance exist. Considering panel (b), if exactly one  $(x^i, y^i)$  lies in each of the gray regions, here the two partially obscured regions with smaller  $x_1$  value are just translated copies of the two top regions, then the four tuples are discordant; again, other types of discordance exist. Unlike in the bivariate case, points may be simultaneously concordant and discordant with respect to  $\tau_P^*$ .

let

$$w^{i_1, \dots, i_m} = w^{(i_1, \dots, i_m)} = (w^{i_1}, \dots, w^{i_m}),$$

$$(w^{i_1, \dots, i_m}, w^{j_1, \dots, j_k}) = (w^{i_1}, \dots, w^{i_m}, w^{j_1}, \dots, w^{j_k}).$$

If  $[n]$  appears in the superscript of a vector it should be interpreted as an ordered vector, that is, we let  $w^{[n]} = w^{(1, \dots, n)} = (w^1, \dots, w^n)$ .

We will state a number of basic definitions and facts regarding groups; for more details see any introductory text on the topic, for instance, Dummit and Foote (2004). We will be primarily interested in the group of permutations.

**Definition 4.4** (Symmetric Group). For any  $n \geq 1$  let  $S_n$  be the collection of all bijective functions  $\sigma : [n] \rightarrow [n]$ . The elements of  $S_n$  represent permutations of  $[n]$ . The set  $S_n$  along with the composition operation  $\circ : S_n \times S_n \rightarrow S_n$  defined by  $(\sigma \circ \gamma)(i) = \sigma(\gamma(i))$  is a group, called the *symmetric group on  $n$  elements*, whose identity element  $e$  is the identity function, i.e.  $e(i) = i$  for all  $i \in [n]$ . We will often omit the  $\circ$  operation and simply write  $\sigma\gamma$  for  $\sigma \circ \gamma$ .

**Definition 4.5** (Cycle). We say that a permutation  $\sigma \in S_n$  is a *cycle of length  $m$*  if there exist distinct  $1 \leq i_1, \dots, i_m \leq n$  such that  $\sigma(i_j) = i_{j+1}$  for  $1 \leq j \leq m-1$ ,  $\sigma(i_m) = i_1$ , and  $\sigma(k) = k$  for any  $k \notin \{i_1, \dots, i_m\}$ . If  $\sigma$  is a cycle as above we write it as  $(i_1 \ i_2 \ \dots \ i_m)$ . Any cycle of length 2 is called a *transposition*.

**Proposition 4.6** (Dummit and Foote (2004)). *Every permutation  $\sigma \in S_n$  can be written as a composition of transpositions. While this decomposition need not be unique, parity of the number of transpositions in any such decomposition is unique. Thus there exists a well-defined function  $\text{sign} : S_n \rightarrow \{-1, 1\}$  such that for any  $\sigma \in S_n$ ,  $\text{sign}(\sigma) = 1$  if  $\sigma$  can be written as the composition of an even number of transpositions and  $\text{sign}(\sigma) = -1$  otherwise.*

We will often observe the symmetric group  $S_n$  acting on vectors  $w^{[n]} \in \mathbb{R}^{d \times n}$ . In such a case we define the (left) group action  $\alpha : S_n \times \mathbb{R}^{d \times n} \rightarrow \mathbb{R}^{d \times n}$  of  $S_n$  on  $\mathbb{R}^{d \times n}$  such that for any  $\sigma \in S_n$  and  $w^{[n]} \in \mathbb{R}^{d \times n}$  we have

$$\alpha(\sigma, w^{[n]}) := \alpha(\sigma, (w^1, \dots, w^n)) := (w^{\sigma^{-1}(1)}, \dots, w^{\sigma^{-1}(n)}).$$

As there is no cause for confusion we will simply write  $\alpha(\sigma, w^{[n]})$  as  $\sigma w^{[n]}$  in the future. To see that the above defines a valid group action note first that clearly  $e w^{[n]} = w^{[n]}$  for all  $w^{[n]} \in \mathbb{R}^{d \times n}$ . Now for any  $\sigma, \gamma \in S_n$  let  $v^{[n]} = \gamma w^{[n]}$  so that

$$\sigma(\gamma w^{[n]}) = \sigma v^{[n]} = (v^{\sigma^{-1}(1)}, \dots, v^{\sigma^{-1}(n)}).$$

We have that  $v^{\sigma^{-1}(i)} = w^j$  for all  $w^{[n]} \in \mathbb{R}^{d \times n}$  if and only if  $\sigma^{-1}(i)$  equals the index of  $\gamma w^{[n]}$  to which  $w^j$  was permuted. That is we must have  $\sigma^{-1}(i) = \gamma(j)$ , inverting we have that  $\gamma^{-1}(\sigma^{-1}(i)) = j$ . Hence we have that

$$\begin{aligned} \sigma(\gamma w^{[n]}) &= \sigma v^{[n]} \\ &= (w^{\gamma^{-1}(\sigma^{-1}(1))}, \dots, w^{\gamma^{-1}(\sigma^{-1}(n))}) \\ &= (w^{(\sigma\gamma)^{-1}(1)}, \dots, w^{(\sigma\gamma)^{-1}(n)}) \\ &= (\sigma\gamma)w^{[n]}. \end{aligned} \tag{4.1}$$

Hence the action we defined is compatible with the group structure of  $S_n$  and hence it is indeed a valid group action.

*Remark 4.7.* In general, we have that

$$\sigma(\gamma w^{[n]}) = \sigma(w^{\gamma^{-1}(1)}, \dots, w^{\gamma^{-1}(n)}) \neq (w^{\sigma^{-1}(\gamma^{-1}(1))}, \dots, w^{\sigma^{-1}(\gamma^{-1}(n))}),$$

notice that this differs from Equation (4.1) as we have  $\sigma^{-1}(\gamma^{-1}(i))$  instead of  $\gamma^{-1}(\sigma^{-1}(i))$ . Intuitively this inequality follows as  $\gamma$  does not “know” that the labels of the  $w^i$  were permuted by  $\gamma$ , it simply acts on the vector  $(w^{\gamma^{-1}(1)}, \dots, w^{\gamma^{-1}(n)})$  as though it was a new vector with sequential labels 1 to  $n$ .

As our contention is that  $[n]$  is a tuple when in the superscript of a vector, we have that  $\sigma w^{[n]} = w^{\sigma[n]}$  for all  $w^{[n]} \in \mathbb{R}^{d \times n}$ . It is, however, important to stress that  $\sigma(1, \dots, n) = (\sigma^{-1}(1), \dots, \sigma^{-1}(n)) \neq (\sigma(1), \dots, \sigma(n))$  in general. We will often write  $w^{\sigma[n]}$  as it is more compact. While letting  $S_n$  act on vectors this way may seem somewhat backwards, the following example shows that it captures the intuition that  $\sigma(i) = j$  means that  $\sigma$  sends the  $i$ th element of a tuple to the  $j$ th position.

**Example 4.8.** Let  $w^{[4]} \in \mathbb{R}^4$ . Then let  $\sigma = (1\ 2\ 3\ 4) \in S_4$  be the permutation that cyclically rotates all elements one entry to the right, that is we have  $\sigma(1) = 2$ ,  $\sigma(2) = 3$ ,  $\sigma(3) = 4$  and  $\sigma(4) = 1$ . Note that  $\sigma^{-1} = (4\ 3\ 2\ 1)$  with  $\sigma^{-1}(4) = 1$ ,  $\sigma^{-1}(3) = 2$ ,  $\sigma^{-1}(2) = 1$  and  $\sigma^{-1}(1) = 4$ . Then we have that

$$\begin{aligned}\sigma w^{[4]} &= (w^{\sigma^{-1}(1)}, w^{\sigma^{-1}(2)}, w^{\sigma^{-1}(3)}, w^{\sigma^{-1}(4)}) \\ &= (w^4, w^1, w^2, w^3) \\ &= w^{4,1,2,3}.\end{aligned}$$

Hence we see that  $\sigma w^{[4]}$  appropriately rotates the entries of  $w^{[4]}$  to the right.

## 4.2 Hoeffding's $D$

A multivariate version of Hoeffding's  $D$  is naturally defined by letting

$$D(X, Y) := \int_{\mathbb{R}^r \times \mathbb{R}^s} \{F_{XY}(x, y) - F_X(x)F_Y(y)\}^2 dF_{XY}(x, y).$$

Since  $X \perp\!\!\!\perp Y$  if and only if  $F_{XY}(x, y) = F_X(x)F_Y(y)$  for all  $x, y$ , it is clear that  $X \perp\!\!\!\perp Y$  implies  $D(X, Y) = 0$ . The converse need not always be true, as the next example shows.

**Example 4.9.** Let  $Z = (X, Y)$  be a bivariate distribution with  $P(X = 1, Y = 0) = P(X = 0, Y = 1) = 1/2$ . Then clearly  $X$  and  $Y$  are not independent but

$$\begin{aligned}D(X, Y) &= \frac{1}{2}\{F_{XY}(1, 0) - F_X(1)F_Y(0)\}^2 + \frac{1}{2}\{F_{XY}(0, 1) - F_X(0)F_Y(1)\}^2 \\ &= \frac{1}{2}(1/2 - 1/2)^2 + \frac{1}{2}(1/2 - 1/2)^2 \\ &= 0.\end{aligned}$$

Thus,  $D(X, Y)$  is I-consistent but not D-consistent in general. It is, however, consistent for a large class of continuous distributions.

**Theorem 4.10** (Multivariate version of Theorem 3.1 in Hoeffding, 1948). *Suppose  $X$  and  $Y$  have a continuous joint density  $f_{XY}$  and continuous marginal densities  $f_X$  and  $f_Y$ . Then  $D(X, Y) = 0$  if and only if  $X \perp\!\!\!\perp Y$ .*

*Proof.* The bivariate case is treated in Theorem 3.1 in Hoeffding (1948). The proof of the multivariate case is analogous.  $\square$

Example 4.9 highlights that the failure of  $D(X, Y)$  to detect all dependence structures can be attributed to the measure of integration  $dF_{XY}$ . This suggests the following modification of  $D$ , which we call Hoeffding's  $R$ ,

$$R(X, Y) = \int_{\mathbb{R}^{r+s}} \{F_{XY}(x, y) - F_X(x)F_Y(y)\}^2 \prod_{i=1}^r dF_{X_i}(x_i) \prod_{j=1}^s dF_{Y_j}(y_j).$$

We suspect that it is well-known that  $R$  is consistent but we could not find a compelling reference of this fact. For completeness we include a proof in Appendix B.

**Theorem 4.11.** *Let  $(X, Y)$  be drawn from a multivariate distribution on  $\mathbb{R}^r \times \mathbb{R}^s$ . Then  $R(X, Y) \geq 0$  and  $R(X, Y) = 0$  if and only if  $X \perp\!\!\!\perp Y$ .*

### 4.3 Bergsma–Dassios Sign-Covariance $\tau^*$

Bergsma and Dassios (2014) defined  $\tau^*$  only for bivariate distributions, so let  $r = s = 1$  for this section. While  $\tau^*$  has a natural definition in terms of concordant and discordant quadruples of points, we will present an alternative definition that will be more useful for our purposes. First for any  $w^{[4]} \in \mathbb{R}^4$  let  $I_{\tau^*}(w^{[4]}) = 1_{(w^1, w^2 < w^3, w^4)}$  where  $w^1, w^2 < w^3, w^4$  if and only if  $\max(w^1, w^2) < \min(w^3, w^4)$ . Then, as is shown by Bergsma and Dassios (2014),

$$\tau^*(X, Y) = E \left[ \left\{ I_{\tau^*}(X^{[4]}) + I_{\tau^*}(X^{4,3,2,1}) - I_{\tau^*}(X^{1,3,2,4}) - I_{\tau^*}(X^{4,2,3,1}) \right\} \right. \\ \left. \left\{ I_{\tau^*}(Y^{[4]}) + I_{\tau^*}(Y^{4,3,2,1}) - I_{\tau^*}(Y^{1,3,2,4}) - I_{\tau^*}(Y^{4,2,3,1}) \right\} \right].$$

While Bergsma and Dassios (2014) conjecture that  $\tau^*$  is consistent for all bivariate distributions, the proof of this statement remains elusive. The current understanding of the consistency of  $\tau^*$  is summarized by the following theorem.

**Theorem 4.12** (Theorem 1 of Bergsma and Dassios, 2014). *Suppose  $(X, Y)$  are drawn from a bivariate continuous distribution, discrete distribution, or a mixture of a continuous and discrete distribution. Then  $\tau^*(X, Y) \geq 0$  and  $\tau^*(X, Y) = 0$  if and only if  $X \perp\!\!\!\perp Y$ .*

Theorem 4.12 does not apply to any singular distributions; for instance, we are not guaranteed that  $\tau^* > 0$  when  $(X, Y)$  are generated uniformly on the unit circle in  $\mathbb{R}^2$ .

## Chapter 5

**SYMMETRIC RANK COVARIANCES: A GENERALISED  
FRAMEWORK FOR NONPARAMETRIC MEASURES OF  
DEPENDENCE**

We now introduce a new class of nonparametric dependence measures that depend on  $X$  and  $Y$  only through their joint ranks.

**Definition 5.1.** Let  $w^{[m]} \in \mathbb{R}^{d \times m}$ . Then the joint rank matrix of  $w^{[m]}$  is the  $[m]$ -valued  $d \times m$  matrix with  $i, j$  entry

$$\mathcal{R}(w^{[m]})_{ij} := 1 + \sum_{k=1}^m \mathbf{1}_{(w_i^k < w_i^j)},$$

that is,  $\mathcal{R}(w^{[m]})_{ij}$  is the rank of  $w_i^j$  among  $w_i^1, \dots, w_i^m$  for  $i \in [d]$ .

**Definition 5.2.** A rank indicator function of order  $m$  and dimension  $d$  is a function  $I : \mathbb{R}^{d \times m} \rightarrow \{0, 1\}$  such that  $I(\mathcal{R}(w^{[m]})) = I(w^{[m]})$  for all  $w^{[m]} \in \mathbb{R}^{d \times m}$ . In other words,  $I$  depends on its arguments only through their joint ranks.

**Definition 5.3.** Let  $I_X$  and  $I_Y$  be rank indicator functions that have equal order  $m$  and are of dimensions  $r$  and  $s$ , respectively. Let  $H$  be a subgroup of the symmetric group  $S_m$  with an equal number of even and odd permutations. Define

$$\mu_{I_X, I_Y, H}(X, Y) := E \left[ \left\{ \sum_{\sigma \in H} \text{sign}(\sigma) I_X(X^{\sigma^{[m]}}) \right\} \left\{ \sum_{\sigma \in H} \text{sign}(\sigma) I_Y(Y^{\sigma^{[m]}}) \right\} \right]. \quad (5.1)$$

Then a measure of dependence  $\mu$  is a *symmetric rank covariance* if there exist a scalar  $c > 0$  and a triple  $(I_X, I_Y, H)$  as specified above such that  $\mu = c \mu_{I_X, I_Y, H}$ . More generally,  $\mu$  is a *summed symmetric rank covariance* if it is the sum of several symmetric rank covariances.

Some of the symmetric rank covariances we consider have the two rank indicator functions equal, so  $I_X = I_Y = I$ . In this case, we also use the abbreviation  $\mu_{I, H} = \mu_{I, I, H}$ .

*Remark 5.4.* In Definition 5.3, the restrictions on  $H$  allow us to both generalise several existing nonparametric measures of dependence and afford us a number of general properties that we leverage in our proofs. An interesting alternative choice, suggested by a referee while this work was under review in the journal *Biometrika*, is to instead let  $H$  be an arbitrary subset of  $S_m$  with some partial order  $\preceq$  for which  $H$  has a unique upper bound denoted  $\widehat{1}$  and unique lower bound denoted  $\widehat{0}$ . When replacing the sign function in Equation (5.1) by the function  $\sigma \mapsto m(\sigma, \widehat{1})$  where  $m : S_m \rightarrow \mathbb{R}$  is the Möbius function corresponding to  $(H, \preceq)$ , one obtains a new collection of measures, which one might naturally call *Möbius rank covariances*, having many of the same properties as the symmetric rank covariances. Indeed, all special cases of symmetric rank covariances considered in this paper are also Möbius rank covariances and one may recover Proposition 5.9 for these measures. While the study of such measures is beyond the scope of this paper, an avenue of future research might consider the properties of such measures when using the lattice structure on  $S_m$  from Duquenne and Cherfouh (1994).

*Remark 5.5.* Recall from Section 4.3 that for any  $z^{[4]} \in \mathbb{R}^4$  we write  $z^1, z^2 < z^3, z^4$  to mean  $\max(z^1, z^2) < \min(z^3, z^4)$ . To simplify the definitions of rank indicator functions we generalise this notation as follows. Let  $\sim$  be any binary relation on  $\mathbb{R}^d$ . Then for  $z^{[l]} \in \mathbb{R}^{d \times l}$  and  $w^{[k]} \in \mathbb{R}^{d \times k}$  we write  $z^1, \dots, z^l \sim w^1, \dots, w^k$  to mean  $z^i \sim w^j$  for all  $(i, j) \in [l] \times [k]$ .

It is easy to show that many existing nonparametric measures of dependence are symmetric rank covariances.

**Proposition 5.6.** *Let  $X$  and  $Y$  take values in  $\mathbb{R}^r$  and  $\mathbb{R}^s$ , respectively. Consider the permutation groups  $H_\tau = \langle (1\ 2) \rangle$  and  $H_{\tau^*} = \langle (1\ 4), (2\ 3) \rangle$ .*

(i) *Bivariate case ( $r = s = 1$ ): Kendall's  $\tau$ , its square  $\tau^2$ , and  $\tau^*$  of Bergsma–Dassios are symmetric rank covariances. Specifically,*

$$\tau := \mu_{I_\tau, H_\tau}, \quad \tau^2 := \mu_{I_{\tau^2}, H_{\tau^2}}, \quad \tau^* := \mu_{I_{\tau^*}, H_{\tau^*}},$$

where the one-dimensional rank indicator functions are defined as

$$I_{\tau^*}(w^{[4]}) := 1_{(w^1, w^2 < w^3, w^4)}, \quad I_{\tau}(w^{[2]}) := 1_{(w^1 < w^2)}, \quad I_{\tau^2}(w^{[4]}) := I_{\tau}(w^{1,4})I_{\tau}(w^{2,3}).$$

(ii) General case ( $r, s \geq 1$ ): Both  $D$  and  $R$  are symmetric rank covariances. Specifically,

$$D = \frac{1}{4} \mu_{I_{D,r}, I_{D,s}, H_{\tau^*}}, \quad R = \frac{1}{4} \mu_{I_{R,r,s,X}, I_{R,r,s,Y}, H_{\tau^*}}$$

where for any  $d \geq 1$  we define

$$\begin{aligned} I_{D,d}(w^{[5]}) &:= 1_{(w^1, w^2 \preceq w^5)} 1_{(w^3, w^4 \not\preceq w^5)} && (w^1, \dots \in \mathbb{R}^d), \\ I_{R,r,s,X}(w^{[4+r+s]}) &:= 1_{\{w^1, w^2 \preceq (w_1^5, \dots, w_r^{4+r})^T\}} 1_{\{w^3, w^4 \not\preceq (w_1^5, \dots, w_r^{4+r})^T\}} && (w^1, \dots \in \mathbb{R}^r), \\ I_{R,r,s,Y}(w^{[4+r+s]}) &:= 1_{\{w^1, w^2 \preceq (w_1^{5+r}, \dots, w_s^{4+r+s})^T\}} 1_{\{w^3, w^4 \not\preceq (w_1^{5+r}, \dots, w_s^{4+r+s})^T\}} && (w^1, \dots \in \mathbb{R}^s) \end{aligned}$$

with  $w^i \preceq w^j$  if and only if  $w_\ell^i \leq w_\ell^j$  for all  $\ell \in [d]$ .

*Remark 5.7.* In Proposition 5.6 we see that, unlike for  $I_{D,d}$ , the length of the input tuples to  $I_{R,r,s,X}, I_{R,r,s,Y}$  grows with  $r$  and  $s$ . While this may seem surprising, it is an immediate consequence of the fact that  $R$  integrates against the product measure  $\prod_{i=1}^r dF_{X_i}(x_i) \prod_{j=1}^s dF_{Y_j}(y_j)$  each component of which requires its own independent observation.

*Remark 5.8.* The bivariate dependence measure Spearman's  $\rho$  can be written as

$$\begin{aligned} \rho(X, Y) = 6 E \Big[ & 1_{(X^1 < X^2 < X^3)} \{ 1_{(Y^1 < Y^2 < Y^3)} + 1_{(Y^1 < Y^3 < Y^2)} + 1_{(Y^2 < Y^1 < Y^3)} \\ & - 1_{(Y^3 < Y^1 < Y^2)} - 1_{(Y^2 < Y^3 < Y^1)} - 1_{(Y^3 < Y^2 < Y^1)} \} \Big]. \end{aligned} \quad (5.2)$$

In light of Lemma 5.11, one might expect  $\rho$  to be a symmetric rank covariance. However, upon examining which of the indicators are negated in (5.2), one notes that the permutations do not respect the sign operation of the permutation group  $S_3$ . For instance,  $1_{(Y^1 < Y^2 < Y^3)}$  and  $1_{(Y^1 < Y^3 < Y^2)}$  are related through a single transposition and yet the terms have the same sign above. While it seems difficult to prove conclusively that  $\rho$  is not a symmetric rank covariance, this suggests that it is not. Somewhat surprisingly however,  $\rho$  is a summed symmetric rank covariance which can be seen by expressing  $\rho$  as

$$\rho(X, Y) = 3 E \left\{ b(X^{[3]})b(Y^{[3]}) + b(X^{[3]})b(Y^{1,3,2}) + b(X^{[3]})b(Y^{2,1,3}) \right\}$$

where  $b(z^{[3]}) = 1_{(z^1 < z^2 < z^3)} - 1_{(z^3 < z^2 < z^1)}$  for all  $z^i \in \mathbb{R}$ .

### 5.1 General Properties

While many interesting properties of symmetric rank covariances depend on the choice of group  $H$  and indicators  $I_X, I_Y$ , several properties hold for all such choices.

**Proposition 5.9.** *Let  $\mu$  be a symmetric rank covariance. Then  $\mu$  is nonparametric and I-consistent. If  $\nu$  is another symmetric rank covariance, then so is the product  $\mu\nu$ .*

*Remark 5.10.* While Proposition 5.9 guarantees that all symmetric rank covariances are nonparametric and I-consistent, showing that such measures are D-consistent must be done on a case-by-case basis and can, in general, be difficult. In Section 5.2 we produce, through a natural generalisation of Hoeffding's  $D$  and  $R$ , a collection of summed symmetric rank covariances for which proving D-consistency is relatively straightforward. Thus Section 5.2 serves to show one strategy by which we may recover D-consistency while also producing a collection of candidate measures for future study.

That symmetric rank covariances are closed under products in particular justifies squaring, as was done for bivariate rank correlations in Leung and Drton (2018). Later, it will be useful to express symmetric rank covariances in an equivalent form.

**Lemma 5.11.** *In reference to Equation (5.1), we have*

$$\mu_{I_X, I_Y, H}(X, Y) = |H| E \left\{ I_X(X^{[m]}) \sum_{\sigma \in H} \text{sign}(\sigma) I_Y(Y^{\sigma[m]}) \right\} \quad (5.3)$$

$$= |H| E \left\{ I_Y(Y^{[m]}) \sum_{\sigma \in H} \text{sign}(\sigma) I_X(X^{\sigma[m]}) \right\}. \quad (5.4)$$

### 5.2 Generalising Hoeffding's $D$ by a Discretization Perspective

This section serves to create a collection of summed symmetric rank covariances, generalising Hoeffding's  $D$  and  $R$ , which are easily seen to be D-consistent. We begin by showing that  $D$  and  $R$  are accumulations of, possibly infinitely many, independence measures between binarized versions of  $X$  and  $Y$ .

**Definition 5.12.** Let  $Z = (Z_1, \dots, Z_d)$  be an  $\mathbb{R}^d$ -valued random vector, and let  $z \in \mathbb{R}^d$ . The binarization of  $Z$  at  $z$  is the random vector

$$B^Z(z) = (1_{(Z_1 > z_1)}, \dots, 1_{(Z_d > z_d)}).$$

We call  $z$  the cutpoint of the binarization.

For any  $z = (x, y) \in \mathbb{R}^{r+s}$  we have  $B^Z(z) = (B^X(x), B^Y(y))$ . Clearly  $B^Z(z)$ ,  $B^X(x)$ ,  $B^Y(y)$  are discrete random variables taking values in  $\{0, 1\}^{r+s}$ ,  $\{0, 1\}^r$ , and  $\{0, 1\}^s$  respectively. The cutpoint  $z$  divides  $\mathbb{R}^r \times \mathbb{R}^s$  into  $2^{r+s}$  orthants corresponding to the states of  $B^Z(z)$ . We index these orthants by vectors  $\ell \in \{0, 1\}^{r+s}$ , and define

$$p(z)_\ell = P(B^Z(z) = \ell) = P(Z_i \underset{\leq \ell_i}{\underset{> \ell_i}{>}} z_i, i \in [r+s]) \quad , \quad \underset{\leq \ell_i}{\underset{> \ell_i}{>}} \equiv \begin{cases} \leq, & \ell_i = 0, \\ >, & \ell_i = 1. \end{cases}$$

Let  $p(z)$  be the  $2 \times \dots \times 2 = 2^{r+s}$  tensor with coordinates  $p(z)_\ell$ . Independence between  $B^X(x)$  and  $B^Y(y)$  can be characterized in terms of the rank of a flattening, or matricization, of  $p(z)$ . Let  $M(x, y)$  be the real  $2^r \times 2^s$  matrix with entries

$$M(x, y)_{\ell_X \ell_Y} = p(z)_{\ell_X \ell_Y}$$

for indices  $\ell_X \in \{0, 1\}^r$ ,  $\ell_Y \in \{0, 1\}^s$  that are concatenated to form  $\ell_X \ell_Y$ . It then holds that  $B^X(x) \perp\!\!\!\perp B^Y(y)$  if and only if  $M(x, y)$  has rank 1 (Drton et al., 2009, Chapter 3).

The matrix  $M(x, y)$  has rank 1 if and only if all of its  $2 \times 2$  minors vanish, that is, for all  $\ell_X, \ell'_X \in \{0, 1\}^r$  and  $\ell_Y, \ell'_Y \in \{0, 1\}^s$  we have

$$\begin{aligned} 0 &= M(x, y)_{\ell_X \ell_Y} M(x, y)_{\ell'_X \ell'_Y} - M(x, y)_{\ell'_X \ell_Y} M(x, y)_{\ell_X \ell'_Y} \\ &= p(z)_{\ell_X \ell_Y} p(z)_{\ell'_X \ell'_Y} - p(z)_{\ell'_X \ell_Y} p(z)_{\ell_X \ell'_Y}. \end{aligned}$$

One may easily show that  $X \perp\!\!\!\perp Y$  if and only if  $B^X(x) \perp\!\!\!\perp B^Y(y)$  for all  $x, y$ . This suggests defining a measure of dependence equal to the integral of the sum of squared minors of the above form. We will need to generalise slightly by considering  $2 \times 2$  block minors defined below. These block minors correspond to the fact that  $B^X(x) \perp\!\!\!\perp B^Y(y)$  if and only

if  $P\{B^X(x) \in L, B^Y(y) \in R\} = P\{B^X(x) \in L\} P\{B^Y(y) \in R\}$  for all  $L \subset \{0, 1\}^r$ ,  $R \subset \{0, 1\}^s$ .

**Definition 5.13.** Let  $L, L' \subset \{0, 1\}^r$  and  $R, R' \subset \{0, 1\}^s$  be nonempty subsets with  $L \cap L' = \emptyset$  and  $R \cap R' = \emptyset$ . Then the  $2 \times 2$  block minor of  $M(x, y)$  along  $(L, L', R, R')$  is the value

$$\begin{aligned} & \left\{ \sum_{\substack{\ell_X \in L \\ \ell_Y \in R}} p(z)_{\ell_X \ell_Y} \right\} \left\{ \sum_{\substack{\ell'_X \in L' \\ \ell'_Y \in R'}} p(z)_{\ell'_X \ell'_Y} \right\} - \left\{ \sum_{\substack{\ell'_X \in L' \\ \ell_Y \in R}} p(z)_{\ell'_X \ell_Y} \right\} \left\{ \sum_{\substack{\ell_X \in L \\ \ell'_Y \in R'}} p(z)_{\ell_X \ell'_Y} \right\} \\ &= \sum_{\substack{\ell_X \in L \\ \ell_Y \in R}} \sum_{\substack{\ell'_X \in L' \\ \ell'_Y \in R'}} \{p(z)_{\ell_X \ell_Y} p(z)_{\ell'_X \ell'_Y} - p(z)_{\ell'_X \ell_Y} p(z)_{\ell_X \ell'_Y}\}. \end{aligned}$$

**Proposition 5.14.**  $B^X(x) \perp\!\!\!\perp B^Y(y)$  if and only if all  $2 \times 2$  block minors of  $M(x, y)$  vanish.

If  $L, L', R, R'$  are singletons the  $2 \times 2$  block minor reduces to a usual  $2 \times 2$  minor.

We now propose to assess dependence by integrating squared block minors. The integration measures we allow are derived from the variables' joint distribution but may be taken to be products of marginals as encountered for the measure of dependence  $R$ .

**Definition 5.15.** For any  $d \geq 0$  let  $0_d \in \mathbb{R}^d$  be the vector of all zeros. A measure  $\mu(X, Y)$  is called an integrated squared minor if there exists  $L \subset \{0, 1\}^r \setminus \{0_r\}$ ,  $R \subset \{0, 1\}^s \setminus \{0_s\}$ ,  $E_1, \dots, E_t$  partitioning  $[r]$ , and  $F_1, \dots, F_t$  partitioning  $[s]$ , such that

$$\mu(X, Y) = \int_{\mathbb{R}^{r+s}} A(x, y)^2 d\lambda_{XY}(x, y)$$

where  $A(x, y)$  is the  $2 \times 2$  block minor of  $M(x, y)$  along  $(\{0_r\}, L, \{0_s\}, R)$ , and the cumulative distribution function  $\lambda_{XY}$  can be written as

$$\lambda_{XY}(x, y) = \prod_{i \in [t]} F_{X_{E_i} Y_{F_i}}(x_{E_i}, y_{F_i}).$$

As the next proposition shows, all integrated squared minor measures are symmetric rank covariances.

**Proposition 5.16.** *Let  $\mu$  be an integrated squared minor as in Definition 5.15, then  $\mu$  is a symmetric rank covariance. In particular, we have  $\mu = \frac{1}{4}\mu_{I_X, I_Y, H}$  where  $H = H_{\tau^*}$  and*

$$\begin{aligned}
I_X(w^{[4+t]}) &= \left\{ \prod_{i \in [t]} 1_{(w_{E_i}^1, w_{E_i}^2 \preceq w_{E_i}^{4+i})} \right\} \left\{ \sum_{\ell^X \in L} \prod_{i \in [t]} \prod_{j \in E_i} 1_{(w_j^3 \stackrel{\leq}{\succ} \ell_j^X w_j^{4+i})} \right\} \\
&\quad \left\{ \sum_{\ell^X \in L} \prod_{i \in [t]} \prod_{j \in E_i} 1_{(w_j^4 \stackrel{\leq}{\succ} \ell_j^X w_j^{4+i})} \right\} && (w^{[4+t]} \in \mathbb{R}^{r \times (4+t)}), \\
I_Y(w^{[4+t]}) &= \left\{ \prod_{i \in [t]} 1_{(w_{F_i}^1, w_{F_i}^2 \preceq w_{F_i}^{4+i})} \right\} \left\{ \sum_{\ell^Y \in R} \prod_{i \in [t]} \prod_{j \in F_i} 1_{(w_j^3 \stackrel{\leq}{\succ} \ell_j^Y w_j^{4+i})} \right\} \\
&\quad \left\{ \sum_{\ell^Y \in R} \prod_{i \in [t]} \prod_{k \in F_i} 1_{(w_k^4 \stackrel{\leq}{\succ} \ell_k^Y w_j^{4+i})} \right\} && (w^{[4+t]} \in \mathbb{R}^{s \times (4+t)}).
\end{aligned}$$

Moreover, if  $L = \{0, 1\}^r \setminus \{0_r\}$  and  $R = \{0, 1\}^s \setminus \{0_s\}$  we have that  $\mu = D$  when  $\lambda_{XY} = F_{XY}$  and  $\mu = R$  when  $\lambda_{XY} = \prod_{i=1}^r F_{X_i} \prod_{j=1}^s F_{Y_j}$ .

Finally we can identify a collection of D-consistent summed symmetric rank covariances.

**Proposition 5.17.** *Let  $L_1, \dots, L_k \subset \{0, 1\}^r \setminus \{0_r\}$  and  $R_1, \dots, R_k \subset \{0, 1\}^s \setminus \{0_s\}$  be two collections of nonempty sets. Suppose that the sets  $L_i \times R_i$  are pairwise disjoint and form a partition of  $(\{0, 1\}^r \setminus \{0_r\}) \times (\{0, 1\}^s \setminus \{0_s\})$ . For all  $i \in [k]$  let*

$$\mu_i^{\text{joint}}(X, Y) = \int_{\mathbb{R}^{r+s}} A_i(x, y)^2 dF_{XY}(x, y)$$

and

$$\mu_i^{\text{prod}}(X, Y) = \int_{\mathbb{R}^{r+s}} A_i(x, y)^2 \prod_{i=1}^r dF_{X_i}(x_i) \prod_{j=1}^s dF_{Y_j}(y_j)$$

where  $A_i(x, y)$  is the  $2 \times 2$  block minor along  $(\{0_r\}, L_i, \{0_s\}, R_i)$ . Then the summed symmetric rank covariance  $\mu^{\text{joint}} = \sum_{i=1}^k \mu_i^{\text{joint}}$  is D-consistent in, at least, all cases that D is; similarly  $\mu^{\text{prod}} = \sum_{i=1}^k \mu_i^{\text{prod}}$  is D-consistent in all cases.

### 5.3 Multivariate $\tau^*$

Recall from Proposition 5.6 that  $\tau^* = \mu_{I_{\tau^*}, H_{\tau^*}}$ . Multivariate extensions of  $\tau^*$  should simultaneously capture essential characteristics while permitting enough flexibility to define

interesting measures of high-order dependence. As a first step to distilling these essential characteristics, it seems natural that any multivariate extension of  $\tau^*$  uses the same permutation subgroup  $H_{\tau^*}$ .

*Remark 5.18.* There are 30 distinct subgroups of  $S_4$  exactly 20 of which have an equal number of even and odd permutations and thus could be used in the definition of a symmetric rank covariance. Given these many possible choices it may seem surprising that  $H_{\tau^*}$  appears in the definition of so many existing measures of dependence, namely  $\tau^*$ ,  $\tau^2$ ,  $D$ , and  $R$ . Some intuition for the ubiquity of  $H_{\tau^*}$  can be gleaned from the proof of Proposition 5.6, see Appendix B.2.2, where we show that  $H_{\tau^*}$  arises naturally from an expansion of  $\{F_{XY}(x, y) - F_X(x)F_Y(y)\}^2$ .

It now remains to find an appropriate generalisation of  $I_{\tau^*}$ . To better characterize  $I_{\tau^*}$  we require the following definition.

**Definition 5.19.** Let  $I$  be a rank indicator function of order  $m$  and dimension  $d$ . The permutations  $\sigma \in S_m$  such that  $I(\sigma w^{[m]}) = I(w^{[m]})$  for all  $w^{[m]} \in \mathbb{R}^{d \times m}$  form a group that we refer to as the *invariance group  $G$  of  $I$* . For any symmetric rank covariance  $\mu_{I_X, I_Y, H}$ , let  $G_X, G_Y$  be the invariance groups of  $I_X$  and  $I_Y$  respectively. We then call  $G = G_X \cap G_Y$  the *invariance group of  $\mu_{I_X, I_Y, H}$* .

We now single out two properties of  $I_{\tau^*}$ :

*Property 5.20.*  $I_{\tau^*}$  is a rank indicator function of order 4;

*Property 5.21.* the invariance group of  $I_{\tau^*}$  is  $\langle (1\ 2), (3\ 4) \rangle$ .

This inspires the following definition.

**Definition 5.22.** A symmetric rank covariance  $\mu_{I_X, I_Y, H}$  is a  $\tau^*$  *extension* if  $I_X$  and  $I_Y$  are rank indicators of order 4 with invariance group  $\langle (1\ 2), (3\ 4) \rangle$  and  $H = H_{\tau^*}$ .

From the possible  $\tau^*$  extensions we consider two notable candidates.

**Definition 5.23.** For any  $d \geq 1$  let  $I_P : \mathbb{R}^{d \times 4} \rightarrow \{0, 1\}$  be the rank indicator, where for any  $w^{[4]} \in \mathbb{R}^{d \times 4}$  we have  $I_P(w^{[4]}) = 1_{(w^3, w^4 \not\prec w^1, w^2)}$ . We then call  $\mu_{I_P, I_P, H_{\tau^*}}$  the multivariate partial  $\tau^*$  and write  $\tau_P^* = \mu_{I_P, I_P, H_{\tau^*}}$ .

The definition of  $I_P$  is inspired by  $I_D$ , see Proposition 5.6.

**Definition 5.24.** For any  $d \geq 1$  let  $I_J : \mathbb{R}^{d \times 4} \rightarrow \{0, 1\}$  be the rank indicator where for any  $w^{[4]} \in \mathbb{R}^{d \times 4}$  we have  $I_J(w^{[4]}) = 1_{(w^1, w^2 \prec w^3, w^4)}$ . We then call  $\mu_{I_J, I_J, H_{\tau^*}}$  the multivariate joint  $\tau^*$  and write  $\tau_J^* = \mu_{I_J, I_J, H_{\tau^*}}$ .

Our definition of  $\tau_J^*$  comes immediately from  $\tau^*$  when replacing the total order  $<$  with  $\prec$ . Although this might be the most intuitive multivariate extension of  $\tau^*$  it is easily seen to not be D-consistent as the next example shows. In both of the above definitions, the extensions reduce to  $\tau^*$  when  $r = s = 1$ .

**Example 5.25.** Let  $X = (X_1, \dots, X_r)$  where  $r$  is even and  $X_1, \dots, X_r \sim \text{Bernoulli}(1/2)$  are independent. Now let  $Y = \text{XOR}(X_1, \dots, X_r)$ , that is, let  $Y = 1$  if  $\sum_{i=1}^r X_i$  is odd and  $Y = 0$  otherwise. Now letting  $(X^i, Y^i)$  be independent and identically distributed replicates of  $(X, Y)$ ,  $I_J(X^{[4]}) = 1$  if and only if  $X^1 = X^2 = (0, \dots, 0)$  and  $X^3 = X^4 = (1, \dots, 1)$ . Thus  $I_J(X^{[4]}) = 1$  implies that  $Y^1 = Y^2 = Y^3 = Y^4 = 0$ , and hence that  $\sum_{\sigma \in H_{\tau^*}} \text{sign}(\sigma) I_J(Y^{\sigma[4]}) = 0$ . Thus we have that  $\tau_J^*(X, Y) = 0$  while  $X \not\prec Y$ .

This behavior only occurs when  $r$  is even. If  $r$  is odd, then  $\tau_J^*(X, Y) = 2^{-4r+2}$ .

Unlike for  $\tau_J^*$ , we have yet to discover an example where  $\tau_P^*(X, Y)$  is 0 when  $X \not\prec Y$ . This leads us to conjecture that  $\tau_P^*$ , like the subclass of measures from Section 5.2, is D-consistent.

## 5.4 Power Simulations

In this section we compare the power of independence tests based on  $D, R, \tau_P^*$ , and  $\tau_J^*$ . As is described in Chapter 6, we may estimate  $D, R, \tau_P^*$ , and  $\tau_J^*$  from data using the U-statistics  $U_D, U_R, U_{\tau_P^*}$ , and  $U_{\tau_J^*}$  respectively. These U-statistics can then be used to test the null hypothesis of independence by rejecting this null hypothesis when the statistics' values are larger

than some critical values. All of the following experiments are run in R (R Core Team, 2018) using the package `SymRC`, which can be obtained from <https://github.com/LucaWeihs/SymRC>. `SymRC` was largely coded in C++ (Stroustrup, 2000) for efficiency.

We will test if a univariate response  $Y$  is independent of a set of covariates  $X = (X_1, \dots, X_r)$ . As explicit asymptotic distributions for  $U_D, U_R, U_{\tau_P^*}$ , and  $U_{\tau_j^*}$  are not known, we will use permutation tests. Unfortunately the computational complexities of  $U_R, U_{\tau_P^*}$ , and  $U_{\tau_j^*}$  are such that, while it is possible to perform permutation tests for a single moderately sized sample, it becomes computationally prohibitive to perform the many thousand tests needed for Monte Carlo approximation of power. We thus approximate the results of permutation tests: first we create a reference distribution for our U-statistic of interest under  $X \perp\!\!\!\perp Y$  by, for  $R = 1000$  replications, randomly generating  $x^1, \dots, x^n$  independently from the marginal distribution of  $X$  and  $y^1, \dots, y^n$  independently from the marginal distribution of  $Y$  and saving the value of the U-statistic for this data set. For an independent and identically distributed sample  $\mathcal{D} = \{(\bar{x}^1, \bar{y}^1), \dots, (\bar{x}^n, \bar{y}^n)\}$  from the true joint distribution of  $(X, Y)$  we then compute a p-value as the proportion of observations in the reference distribution that are greater or equal to the value of the U-statistic when computed on  $\mathcal{D}$ .

This procedure differs from a standard permutation test only in that the reference distribution, and hence critical value for rejection, differ slightly. Empirical tests using small samples suggest, however, that results using the above procedure generalise well to those when using a true permutation test. Computing  $U_D$  is sufficiently fast that we do not need to use the above procedure and instead use a standard permutation test.

For comparison, we also compute the power of the permutation test based on the distance covariance  $d_{\text{cov}}$  as computed by the `energy` package in R (Rizzo and Szekely, 2016). While  $d_{\text{cov}}$  is not a nonparametric measure, we can create a nonparametric version of it by instead considering the measure  $d_{\text{cov}}^{\text{rank}} = d_{\text{cov}}\{(F_{X_1}[X_1], \dots, F_{X_r}[X_r]), (F_{Y_1}[Y_1], \dots, F_{Y_s}[Y_s])\}$ , we also compute the power of a test based on this measure. Of course, in practice, we do not know  $F_{X_1}, \dots, F_{Y_s}$  and thus must estimate them with the marginal empirical cumulative distribution functions. In each of our simulations, we estimate the power using 1000 sample

data sets from the relevant joint distribution.

We consider two cases in which we generate samples of size 50 from jointly continuous distributions. First, we let  $r = 2$ ,  $X_1, X_2$  be independent samples from a  $N(0, 1)$  distribution, and  $Y = X_1 X_2 + \epsilon$  where  $\epsilon \sim N(0, \sigma^2)$ , with  $\sigma \in \{0, \dots, 5\}$ . Figure 5.1a depicts the power of the tests of the hypothesis that  $X \perp\!\!\!\perp Y$ . For comparison, we have also included the power of the distance covariance when  $Y$  has been monotonically transformed by the function  $f(y) = \text{sign}(y) \log(|y| + 10)$ , this transformation substantially reduces the power of the distance covariance while it would have no impact on the power of the other tests as they are nonparametric. In the second case we let  $X_1, X_2$  and  $\epsilon$  be as above but define  $Y = \exp\{-(X_1 - X_2)^2\} + \epsilon$ . Figure 5.1b displays the power of the tests as  $\sigma$  varies in  $\{0, \dots, 2\}$ . The power of the test based on  $\tau_j^*$  is always near the nominal 0.05 level, suggesting that  $\tau_j^*(X, Y) = 0$  and thus that  $\tau_j^*$  is not D-consistent in this case.

We also consider two cases in which  $(X, Y)$  is generated from a jointly discrete distribution. Unlike in the continuous case, the sample size  $n$  will vary with  $n \in \{16, 20, \dots, 48\}$ . Firstly, we let  $r = 2$ ,  $X_1, X_2$  be independent samples from a Bernoulli(1/2) distribution, and  $Y = \text{XOR}(X_1, X_2)$ . We compute the power of our tests for various sample sizes and plot the results in Figure 5.2a. As we would expect from Example 5.25, the power of the test based on  $\tau_j^*$  equals 0 at all sample sizes. Secondly, we let  $r = 3$ ,  $X_1, X_2, X_3$  be independent samples from a Bernoulli(1/2) distribution, and define  $Y = \text{XOR}(X_1, X_2, X_3)$ . Figure 5.2b displays the power of the tests in this setting. Unlike in the prior case, the power of the test based on  $\tau_j^*$  is quite high; again recall from Example 5.25 that this is because  $r$  is odd.

We conclude with a mixed case, where the covariates  $X_1, X_2$  are continuous but the response,  $Y$ , is binary. In particular, we let  $X_1, X_2$  be independent  $N(0, 1)$  while  $Y \sim \text{Bernoulli}[\text{expit}\{6 \sin(X_1 X_2)\}]$ . Empirical power computations are displayed in Figure 5.3.

No independence test dominates the others in our simulations. The fact that the nonparametric tests often perform nearly as well, or better, than the distance covariance is surprising, however, as they are invariant to such a wide range of transformations. Indeed  $d_{\text{cov}}^{\text{rank}}$  never performs substantially worse than  $d_{\text{cov}}$  in our experiments. While it is certainly

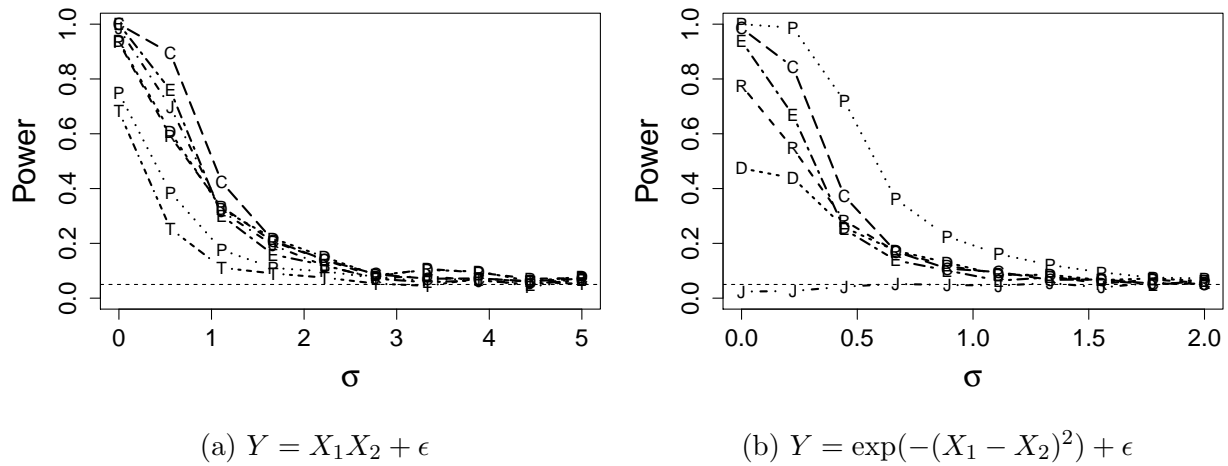


Figure 5.1: Empirical power of permutation tests using  $U_D$  (small dashed line with symbol D),  $U_R$  (medium dashed, R),  $U_{\tau_P^*}$  (dotted, P),  $U_{\tau_J^*}$  (dashed and dotted, J),  $d_{\text{cov}}$  (long dashed, C), and  $d_{\text{cov}}^{\text{rank}}$  (small and long dashes, E), in the continuous case. The fine horizontal line shows the nominal 0.05 level. Here  $\sigma$  is the standard deviation of the additive noise  $\epsilon$ . For Figure 5.1a, the line with symbol T, corresponds to  $d_{\text{cov}}$  after applying the strictly increasing transformation  $y \mapsto \text{sign}(y) \log(|y| + 10)$  to  $Y$ .

not a proof, the fact that the tests based on  $\tau_P^*$  have power beyond the nominal level in all cases suggests that, unlike  $\tau_J^*$ , perhaps  $\tau_P^*$  is indeed D-consistent.

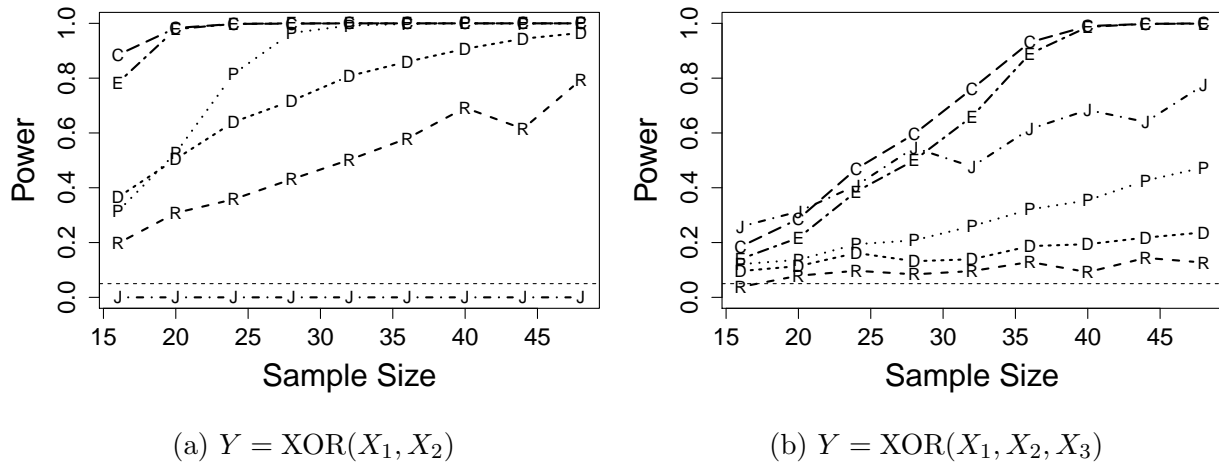


Figure 5.2: Empirical power of permutation tests of independence for a jointly discrete distribution when  $n \in \{16, 20, \dots, 48\}$ . See Figure 5.1 for the correspondence between line and test.

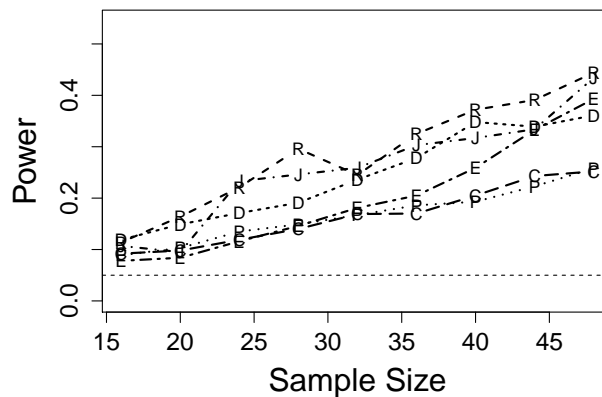


Figure 5.3: Empirical power of permutation tests of independence when  $n \in \{16, 20, \dots, 48\}$ . Here  $Y \sim \text{Bernoulli}[\text{expit}\{6 \sin(X_1 X_2)\}]$  so the joint distribution  $(X, Y)$  is neither jointly continuous nor jointly discrete. See Figure 5.1 for the correspondence between line and test.

## Chapter 6

## COMPUTATIONALLY EFFICIENT ESTIMATION

Symmetric rank covariances can be readily estimated using U-statistics. As naïvely computing these U-statistics is often intractable, we will show how efficient data structures from computational geometry can often be used to substantially decrease run-time.

Let  $\mu = \mu_{I_X, I_Y, H}$  be as in equation (5.1). We let  $\kappa : \mathbb{R}^{(r+s) \times m} \rightarrow \mathbb{R}$  be the *symmetrized kernel function* defined by

$$\kappa(z^1, \dots, z^m) := \frac{1}{m!} \sum_{\sigma \in S_m} k(z^{\sigma[m]}) \quad (6.1)$$

where the *unsymmetrized kernel function*  $k : \mathbb{R}^{(r+s) \times m} \rightarrow \mathbb{R}$  is defined by

$$k(z^{[m]}) := \left\{ \sum_{\sigma \in H} \text{sign}(\sigma) I_X(x^{\sigma[m]}) \right\} \left\{ \sum_{\sigma \in H} \text{sign}(\sigma) I_Y(y^{\sigma[m]}) \right\}.$$

Then we define, for  $n \geq m$  and  $z^{[n]} \in \mathbb{R}^{d \times n}$ ,

$$U_\mu(z^{[n]}) := \frac{1}{\binom{n}{m}} \sum_{1 \leq i_1 < \dots < i_m \leq n} \kappa(z^{i_1, \dots, i_m}). \quad (6.2)$$

We call  $U_\mu$  the *U-statistic corresponding to  $\mu$* . Clearly,  $U_\mu(Z^{[n]})$  is unbiased for  $\mu(X, Y)$ . For computational friendliness we will sometimes rewrite  $\kappa$  using the following proposition.

**Proposition 6.1.** *For any  $z^{[m]} \in \mathbb{R}^{d \times m}$*

$$\kappa(z^{[m]}) = \frac{|H|}{m!} \sum_{\gamma \in S_m} I_X(x^{\gamma[m]}) \sum_{\sigma \in H} \text{sign}(\sigma) I_Y(y^{\sigma\gamma[m]}) \quad (6.3)$$

$$= \frac{|H|}{m!} \sum_{\gamma \in S_m} I_Y(y^{\gamma[m]}) \sum_{\sigma \in H} \text{sign}(\sigma) I_X(X^{\sigma\gamma[m]}). \quad (6.4)$$

### 6.1 Efficient Computation via Orthogonal Range Queries

The U-statistics defined by Equation (6.2) are a sum over  $n$  choose  $m$  many elements and thus, assuming the indicator functions  $I_X, I_Y$  can be computed in  $m$  time, require  $O(m \binom{n}{m})$  operations in a naïve computation. While this may be feasible for small  $m$  and  $n$ , it will be prohibitive for even moderate sample sizes. While subsampling can be used to approximate our statistics of interest, it is not always clear how many samples of which size should be taken to obtain acceptable approximation error and, when many such samples are needed, subsampling approximations need not be fast. Fortunately, when specializing to the U-statistics estimating  $D, R, \tau_P^*$ , and  $\tau_J^*$ , we show that the use of efficient data structures from computational geometry can reduce the asymptotic run-time of the computations. While our observations do not generalise to all symmetric rank covariances, there appear to be many, for instance  $\tau^2$ , for which a similar approach can be used to reduce run-time. For very large samples, these computational strategies could be combined with subsampling procedures to more rapidly achieve low approximation error.

For the remainder of this section we assume that we have observed data  $z^{[n]} \in \mathbb{R}^{d \times n}$ . Moreover, to simplify our run-time analyses, we will assume that  $d$  is bounded, so that for any functions  $f, g : \mathbb{N} \rightarrow \mathbb{N}$  and  $h : \mathbb{N}^2 \rightarrow \mathbb{N}$  we have that  $O\{f(d)+g(d)h(n, d)\} = O\{h(n, d)\}$ .

As the above-defined U-statistics depend on  $z^{[n]}$  only through their joint ranks, we will make the further assumption that  $z^{[n]} = \mathcal{R}(z^{[n]}) \in [n]^{d \times n}$  so that we have transformed  $z^{[n]}$  into its corresponding matrix of joint ranks. The computational effort of this procedure is  $O\{n \log_2(n)\}$  and, as none of the algorithms we will present run in time less than this, performing this preprocessing step does not change the overall analysis.

In the bivariate case, it follows easily from the discussion by Hoeffding (1948) that  $D$  can be computed in  $O(n \log_2 n)$  time while, more recently, it has been shown that  $\tau^*$  can be computed in  $O(n^2)$  time (Heller and Heller, 2016; Weihs et al., 2016). These computational savings largely rely on the ability to efficiently perform orthogonal range queries.

**Definition 6.2.** Let  $z^{[n]} \in \mathbb{R}^{d \times n}$ . Then the question, how many  $z^i$  lie in  $B \subset \mathbb{R}^d$ ?, is an

orthogonal range query on  $\{z^1, \dots, z^n\}$  if  $B = I_1 \times \dots \times I_d$  and, for  $1 \leq i \leq d$ ,  $I_i$  is an interval of the form  $(l_i, u_i)$ ,  $[l_i, u_i)$ ,  $(l_i, u_i]$ , or  $[l_i, u_i]$  for some  $l_i, u_i \in \mathbb{R}$ .

As the next proposition shows using a simple dynamic programming approach one may easily construct an  $n^d$  tensor so that any orthogonal range query on  $z^{[n]}$  can be answered in  $O(1)$  time. See Heller and Heller (2016) for the bivariate case.

**Proposition 6.3.** *Let  $z^{[n]} \in \mathbb{R}^{d \times n}$  be such that  $z^{[n]} = \mathcal{R}(z^{[n]})$ . Then let  $A \in \mathbb{N}^{(n+1) \times \dots \times (n+1)}$  be a  $d$ -dimensional tensor indexed by elements of  $\{0, \dots, n\}^d$  with  $(i_1, \dots, i_d) \in \{0, \dots, n\}^d$  entry equaling*

$$A(i_1, \dots, i_d) = \sum_{i=1}^n 1_{\{z^i=(i_1, \dots, i_d)\}}$$

so that  $A(i_1, \dots, i_d)$  equals the number of elements  $z^i$  with value  $(i_1, \dots, i_d)$ . Now define  $B \in \mathbb{N}^{(n+1) \times \dots \times (n+1)}$  recursively so that it has  $(i_1, \dots, i_d) \in \{0, \dots, n\}^d$  entry  $B(i_1, \dots, i_d) = 0$  if any  $i_j = 0$  and otherwise

$$B(i_1, \dots, i_d) = A(i_1, \dots, i_d) + \sum_{s=1}^d \sum_{\substack{\ell \in \{0,1\}^d \setminus \{0_d\} \\ \sum_k \ell_k = s}} (-1)^{s+1} B\{(i_1, \dots, i_d) - \ell\}.$$

Then for any  $l = (l_1, \dots, l_d), u = (u_1, \dots, u_d) \in \{0, \dots, n\}^d$  the answer to the orthogonal range query, how many  $z^i$  lie in  $B = (l_1, u_1] \times \dots \times (l_d, u_d]?$ , equals

$$\sum_{\ell \in \{0,1\}^d} (-1)^{\sum_{j=1}^d \ell_j} B(l_1^{\ell_1} u_1^{1-\ell_1}, \dots, l_d^{\ell_d} u_d^{1-\ell_d}).$$

When  $d$  is bounded and  $B$  is given, the above sum takes  $O(1)$  time to compute.

*Proof.* This follows by application of the inclusion-exclusion principle. □

Unfortunately, the above tensor takes  $O(n^d)$  time to construct, so, when  $d \geq m$  this procedure already takes at least as long as computing the U-statistic naïvely. In such cases, the range-tree data structure provides a better balance between quickly computing orthogonal range queries and the effort required for its construction.

**Proposition 6.4** (Range-Tree Data Structure, de Berg et al., 2008). *Let  $z^{[n]} \in \mathbb{R}^{d \times n}$ . There exists a data structure, called a range-tree, which takes  $O\{n \log_2(n)^{d-1}\}$  time to construct and can answer any orthogonal range query on  $z^{[n]}$  in  $O\{\log_2(n)^{d-1}\}$  time.*

See Section 5 of de Berg et al. (2008) for a detailed exposition on range-trees, along with a discussion of the above proposition, and orthogonal range queries in general. As, to the best of our knowledge, there exists no open source, completely general, implementation of range-trees, we make such an implementation freely available.<sup>1</sup> Range-trees are closely related to binary search trees, such as red-black trees, which have been previously used to efficiently compute the U-statistics corresponding to  $\tau$  and  $\tau^*$  (Christensen, 2005; Weihs et al., 2016). Using these data structures we obtain substantial run-time savings.

**Proposition 6.5.** *When using the algorithms described in Section 6.2, 6.3, and 6.4, the asymptotic run-times of computing  $U_D, U_R, U_{\tau_P^*}$ , and  $U_{\tau_J^*}$  are  $O\{n \log_2(n)^{d-1}\}$ ,  $O(n^d)$ ,  $O\{n^2 \log_2(n)^{2d-1}\}$ , and  $O\{n^2 \log_2(n)^{2d-1}\}$  respectively. When computing these statistics naïvely their asymptotic run-times are  $O(n^5)$ ,  $O(n^{4+d})$ ,  $O(n^4)$ , and  $O(n^4)$  respectively.*

## 6.2 Computing $U_D$

In this section we will show how to compute  $U_D$  in  $O\{n \log(n)^{d-1}\}$  time. By Proposition 6.1 we have that

$$\begin{aligned} \kappa^D(z^{[5]}) &= \frac{1}{5!} \sum_{\gamma \in S_m} \frac{1}{4} \left\{ \sum_{\sigma \in H_{\tau^*}} \text{sign}(\sigma) I_D(x^{\sigma\gamma^{[5]}}) \right\} \left\{ \sum_{\sigma \in H_{\tau^*}} \text{sign}(\sigma) I_D(y^{\sigma\gamma^{[5]}}) \right\} \\ &= \frac{1}{5!} \sum_{\gamma \in S_m} \frac{|H_{\tau^*}|}{4} I_D(x^{\gamma^{[5]}}) \left\{ \sum_{\sigma \in H_{\tau^*}} \text{sign}(\sigma) I_D(y^{\sigma\gamma^{[5]}}) \right\} \\ &= \frac{1}{5!} \sum_{\gamma \in S_m} I_D(x^{\gamma^{[5]}}) \left\{ \sum_{\sigma \in H_{\tau^*}} \text{sign}(\sigma) I_D(y^{\sigma\gamma^{[5]}}) \right\}. \end{aligned}$$

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<sup>1</sup>See <https://github.com/LucaWeihs/range-tree>

Recalling the definition of  $I_D$  this gives

$$\begin{aligned}
U_D(z^{[n]}) &= \frac{1}{\binom{n}{5}5!} \sum_{\substack{1 \leq i_1, \dots, i_5 \leq n \\ i_1 \neq i_2 \neq \dots \neq i_5}} \mathbf{1}_{(x^{i_1}, x^{i_2} \preceq x^{i_5})} \mathbf{1}_{(x^{i_3}, x^{i_4} \not\preceq x^{i_5})} \\
&\quad \cdot \left\{ \mathbf{1}_{(y^{i_1}, y^{i_2} \preceq y^{i_5})} \mathbf{1}_{(y^{i_3}, y^{i_4} \not\preceq y^{i_5})} + \mathbf{1}_{(y^{i_4}, y^{i_3} \preceq y^{i_5})} \mathbf{1}_{(y^{i_2}, y^{i_1} \not\preceq y^{i_5})} \right. \\
&\quad \left. - \mathbf{1}_{(y^{i_1}, y^{i_3} \preceq y^{i_5})} \mathbf{1}_{(y^{i_2}, y^{i_4} \not\preceq y^{i_5})} - \mathbf{1}_{(y^{i_4}, y^{i_2} \preceq y^{i_5})} \mathbf{1}_{(y^{i_3}, y^{i_1} \not\preceq y^{i_5})} \right\}.
\end{aligned}$$

Now for any  $1 \leq k \leq n$  define

$$\begin{aligned}
C_{\preceq, \preceq}(k) &:= |\{i : i \neq k \text{ and } x^i \preceq x^k \text{ and } y^i \preceq y^k\}| \\
&= |\{i : z^i \preceq z^k\}| - 1 \\
C_{\preceq, \not\preceq}(k) &:= |\{i : i \neq k \text{ and } x^i \preceq x^k \text{ and } y^i \not\preceq y^k\}| \\
&= |\{i : x^i \preceq x^k\}| - |\{i : z^i \preceq z^k\}|, \\
C_{\not\preceq, \preceq}(k) &:= |\{i : i \neq k \text{ and } x^i \not\preceq x^k \text{ and } y^i \preceq y^k\}| \\
&= |\{i : y^i \preceq y^k\}| - |\{i : z^i \preceq z^k\}|, \\
C_{\not\preceq, \not\preceq}(k) &:= |\{i : i \neq k \text{ and } x^i \not\preceq x^k \text{ and } y^i \not\preceq y^k\}| \\
&= n - |\{i : x^i \preceq x^k\}| - |\{i : y^i \preceq y^k\}| + |\{i : z^i \preceq z^k\}|.
\end{aligned}$$

From this, for fixed  $i_5$ ,

$$\begin{aligned}
&\sum_{\substack{1 \leq i_1, \dots, i_4 \leq n \\ i_1 \neq i_2 \neq \dots \neq i_5}} \mathbf{1}_{(x^{i_1}, x^{i_2} \preceq x^{i_5})} \mathbf{1}_{(x^{i_3}, x^{i_4} \not\preceq x^{i_5})} \mathbf{1}_{(y^{i_1}, y^{i_2} \preceq y^{i_5})} \mathbf{1}_{(y^{i_3}, y^{i_4} \not\preceq y^{i_5})} \\
&= |\{\text{pairs } i \neq j \text{ with } i \neq i_5 \neq j \text{ and } z^i, z^j \preceq z^{i_5}\}| |\{\text{pairs } i, j \text{ with } x^i, x^j \not\preceq x^{i_5} \text{ and } y^i, y^j \not\preceq y^{i_5}\}| \\
&= 4 \binom{C_{\preceq, \preceq}(i_5)}{2} \binom{C_{\not\preceq, \not\preceq}(i_5)}{2} \\
&= A(i_5).
\end{aligned}$$

Similarly we have

$$\begin{aligned}
& \sum_{\substack{1 \leq i_1, \dots, i_4 \leq n \\ i_1 \neq i_2 \neq \dots \neq i_5}} \mathbf{1}_{(x^{i_1}, x^{i_2} \preceq x^{i_5})} \mathbf{1}_{(x^{i_3}, x^{i_4} \not\preceq x^{i_5})} \mathbf{1}_{(y^{i_4}, y^{i_3} \preceq y^{i_5})} \mathbf{1}_{(y^{i_2}, y^{i_1} \not\preceq y^{i_5})} \\
&= |\{\text{pairs } i, j \text{ with } x^i, x^j \preceq x^{i_5} \text{ and } y^i, y^j \not\preceq y^{i_5}\}| \cdot |\{\text{pairs } i, j \text{ with } x^i, x^j \not\preceq x^{i_5} \text{ and } y^i, y^j \preceq y^{i_5}\}| \\
&= 4 \binom{C_{\preceq, \not\preceq}(i_5)}{2} \binom{C_{\not\preceq, \preceq}(i_5)}{2} \\
&= B(i_5),
\end{aligned}$$

and

$$\begin{aligned}
& \sum_{\substack{1 \leq i_1, \dots, i_4 \leq n \\ i_1 \neq i_2 \neq \dots \neq i_5}} \mathbf{1}_{(x^{i_1}, x^{i_2} \preceq x^{i_5})} \mathbf{1}_{(x^{i_3}, x^{i_4} \not\preceq x^{i_5})} \mathbf{1}_{(y^{i_1}, y^{i_3} \preceq y^{i_5})} \mathbf{1}_{(y^{i_2}, y^{i_4} \not\preceq y^{i_5})} \\
&= \sum_{\substack{1 \leq i_1, \dots, i_4 \leq n \\ i_1 \neq i_2 \neq \dots \neq i_5}} \mathbf{1}_{(x^{i_1}, x^{i_2} \preceq x^{i_5})} \mathbf{1}_{(x^{i_3}, x^{i_4} \not\preceq x^{i_5})} \mathbf{1}_{(y^{i_4}, y^{i_2} \preceq y^{i_5})} \mathbf{1}_{(y^{i_3}, y^{i_1} \not\preceq y^{i_5})} \\
&= C_{\preceq, \preceq}(i_5) C_{\not\preceq, \not\preceq}(i_5) C_{\preceq, \preceq}(i_5) C_{\not\preceq, \not\preceq}(i_5) \\
&= C(i_5).
\end{aligned}$$

Thus we have that

$$U_D(z^1, \dots, z^n) = \frac{1}{\binom{n}{5} 5!} \sum_{1 \leq i \leq n} \{A(i) + B(i) - 2 C(i)\}. \quad (6.5)$$

Now it is easy to verify that, for any  $1 \leq i \leq n$ , we may compute  $A(i)$ ,  $B(i)$ , and  $C(i)$  using a constant number of orthogonal range queries on  $z^{[n]}$ . Noting that it takes  $O\{n \log_2(n)^{d-1}\}$  to construct the range-tree on  $z^{[n]}$ , each orthogonal range query takes  $O\{\log_2(n)^{d-1}\}$  time, and there are  $n$  iterations in the above sum, it follows that we may compute  $U_D(z^1, \dots, z^n)$  in  $O\{n \log_2(n)^{d-1}\} + n O\{\log_2(n)^{d-1}\} = O\{n \log_2(n)^{d-1}\}$  time.

### 6.3 Computing $U_R$

Recall that the kernel  $\kappa^R$  is of order  $m = d+4$  and so naively takes  $O(n^{d+4})$  time to compute, we will show that it can be computed in  $O(n^d)$  time. By similar arguments as in Section 6.2

we have that

$$U_R(z^{[n]}) = \frac{1}{\binom{n}{m} m!} \sum_{\substack{i^{[d]} = (i^1, \dots, i^d) \in [n]^d \\ i^1 \neq \dots \neq i^d}} \{A^R(i^{[d]}) + B^R(i^{[d]}) - 2 C^R(i^{[d]})\} \quad (6.6)$$

where

$$\begin{aligned} A^R(i^{[d]}) &:= 4 \binom{C_{\leq, \leq}^R(i^{[d]})}{2} \binom{C_{\geq, \geq}^R(i^{[d]})}{2}, \\ B^R(i^{[d]}) &:= 4 \binom{C_{\leq, \geq}^R(i^{[d]})}{2} \binom{C_{\geq, \leq}^R(i^{[d]})}{2}, \\ C^R(i^{[d]}) &:= C_{\leq, \leq}^R(i^{[d]}) C_{\geq, \geq}^R(i^{[d]}) C_{\leq, \geq}^R(i^{[d]}) C_{\geq, \leq}^R(i^{[d]}) \end{aligned}$$

and, letting  $w = (w^X, w^Y) \in \mathbb{R}^{r+s}$  be such that  $w_j^X = x_j^{ij}$  for  $j \in [r]$  and  $w_j^Y = y_j^{ij}$  for  $j \in [s]$ ,

$$\begin{aligned} C_{\leq, \leq}^R(i^{[d]}) &:= |\{i : i \notin \{i^1, \dots, i^d\} \text{ and } x^i \preceq w^X \text{ and } y^i \preceq w^Y\}| \\ &= |\{i : z^i \preceq w\}| - |\{j : z^{ij} \preceq w\}| \\ C_{\leq, \geq}^R(i^{[d]}) &:= |\{i : i \notin \{i^1, \dots, i^d\} \text{ and } x^i \preceq w^X \text{ and } y^i \not\preceq w^Y\}| \\ &= |\{i : x^i \preceq w^X\}| - |\{i : z^i \preceq w\}| - |\{j : x^{ij} \preceq w^X \text{ and } y^{ij} \not\preceq w^Y\}|, \\ C_{\geq, \leq}^R(i^{[d]}) &:= |\{i : i \notin \{i^1, \dots, i^d\} \text{ and } x^i \not\preceq w^X \text{ and } y^i \preceq w^Y\}| \\ &= |\{i : y^i \preceq w^Y\}| - |\{i : z^i \preceq w\}| - |\{j : x^{ij} \not\preceq w^X \text{ and } y^{ij} \preceq w^Y\}|, \\ C_{\geq, \geq}^R(i^{[d]}) &:= |\{i : i \notin \{i^1, \dots, i^d\} \text{ and } x^i \not\preceq w^X \text{ and } y^i \not\preceq w^Y\}| \\ &= n - |\{i : x^i \preceq w^X\}| - |\{i : y^i \preceq w^Y\}| + |\{i : z^i \preceq w\}| \\ &\quad - |\{j : x^{ij} \not\preceq w^X \text{ and } y^{ij} \not\preceq w^Y\}|. \end{aligned}$$

Clearly each of  $A^R(i^{[d]})$ ,  $B^R(i^{[d]})$ , and  $C^R(i^{[d]})$  can be computed using a constant number of orthogonal range searches. Now, constructing the tensor from Proposition 6.3 for  $z^{[n]}$  takes  $O(n^d)$  time after which orthogonal range searches on  $z^{[n]}$  can be completed in constant time. The summation in Equation (6.6) is over  $n^d$  elements and thus, using the tensor, the summation can be completed in  $O(n^d)$  time. It then follows that the total time to compute  $U_R(z^{[n]})$  is  $O(n^d) + O(n^d) = O(n^d)$  as claimed.

### 6.4 Computing $U_{\tau_J^*}$ and $U_{\tau_P^*}$

The computation of the U-statistics estimating  $\tau_J^*$  and  $\tau_P^*$  is somewhat more involved than that for those estimating  $U_D$  and  $U_R$ . By Proposition 6.1 we have that

$$\kappa^{\tau_P^*}(z^{[4]}) = \frac{1}{3!} \sum_{\gamma \in S_4} I_P(x^{\gamma[4]}) \sum_{\sigma \in H_{\tau^*}} \text{sign}(\sigma) I_J(y^{\sigma\gamma[4]}).$$

This then gives us that

$$\begin{aligned} U_{\tau_J^*}(z^{[n]}) &= \frac{1}{\binom{n}{4} 3!} \sum_{\substack{1 \leq i_1, \dots, i_4 \leq n \\ i_1 \neq \dots \neq i_4}} 1_{(x^{i_3}, x^{i_4} \not\leq x^{i_1}, x^{i_2})} \left\{ 1_{(y^{i_3}, y^{i_4} \not\leq y^{i_1}, y^{i_2})} + 1_{(y^{i_2}, y^{i_1} \not\leq y^{i_4}, y^{i_3})} \right. \\ &\quad \left. - 1_{(y^{i_2}, y^{i_4} \not\leq y^{i_1}, y^{i_3})} - 1_{(y^{i_3}, y^{i_1} \not\leq y^{i_4}, y^{i_2})} \right\} \\ &= \frac{1}{\binom{n}{4} 3!} \sum_{\substack{1 \leq i_1, \dots, i_4 \leq n \\ i_1 \neq \dots \neq i_4}} 1_{(x^{i_3}, x^{i_4} \not\leq x^{i_1}, x^{i_2})} \left\{ 1_{(y^{i_3}, y^{i_4} \not\leq y^{i_1}, y^{i_2})} + 1_{(y^{i_2}, y^{i_1} \not\leq y^{i_4}, y^{i_3})} - 2 \cdot 1_{(y^{i_2}, y^{i_4} \not\leq y^{i_1}, y^{i_3})} \right\} \end{aligned}$$

where the second equality follows by swapping the labels of 1,2 and 3,4 respectively. Similarly as in the prior sections, for fixed  $i_1, i_2$ ,

$$\begin{aligned} &\sum_{\substack{1 \leq i_3, i_4 \leq n \\ i_1 \neq \dots \neq i_4}} 1_{(x^{i_3}, x^{i_4} \not\leq x^{i_1}, x^{i_2})} 1_{(y^{i_3}, y^{i_4} \not\leq y^{i_1}, y^{i_2})} \\ &= |\{\text{pairs } k \neq l \text{ with } k, l \notin \{i_1, i_2\}, x^k, x^l \not\leq x^{i_1}, x^{i_2} \text{ and } y^k, y^l \not\leq y^{i_1}, y^{i_2}\}| \\ &= 2 \binom{n - |\{i : x^i \leq x^{i_1} \text{ or } x^i \leq x^{i_2} \text{ or } y^i \leq y^{i_1} \text{ or } y^i \leq y^{i_2}\}|}{2}. \end{aligned} \quad (6.7)$$

Now, using the standard inclusion-exclusion formulas we may compute  $|\{i : x^i \leq x^{i_1} \text{ or } x^i \leq x^{i_2} \text{ or } y^i \leq y^{i_1} \text{ or } y^i \leq y^{i_2}\}|$  using 16 orthogonal range queries on  $z^{[n]}$ .

Next

$$\begin{aligned} &\sum_{\substack{1 \leq i_3, i_4 \leq n \\ i_1 \neq \dots \neq i_4}} 1_{(x^{i_3}, x^{i_4} \not\leq x^{i_1}, x^{i_2})} 1_{(y^{i_2}, y^{i_1} \not\leq y^{i_4}, y^{i_3})} \\ &= |\{\text{pairs } k \neq l \text{ with } k, l \notin \{i_1, i_2\}, x^k, x^l \not\leq x^{i_1}, x^{i_2}, \text{ and } y^{i_1}, y^{i_2} \not\leq y^k, y^l\}| \\ &= 2 \binom{n - |\{i : x^i \leq x^{i_1} \text{ or } x^i \leq x^{i_2} \text{ or } y^{i_1} \leq y^i \text{ or } y^{i_2} \leq y^i\}|}{2}. \end{aligned} \quad (6.8)$$

Again, by inclusion-exclusion, we have that  $|\{i : x^i \preceq x^{i_1} \text{ or } x^i \preceq x^{i_2} \text{ or } y^{i_1} \preceq y^i \text{ or } y^{i_2} \preceq y^i\}|$  can be computed using 16 orthogonal range queries on  $z^{[n]}$ . We now have the most difficult case remaining. We have that

$$\begin{aligned}
& \sum_{\substack{1 \leq i_3, i_4 \leq n \\ i_1 \neq \dots \neq i_4}} \mathbf{1}_{(x^{i_3}, x^{i_4} \not\preceq x^{i_1}, x^{i_2})} \mathbf{1}_{(y^{i_2}, y^{i_4} \not\preceq y^{i_1}, y^{i_3})} \\
&= |\{\text{pairs } k \neq l \text{ with } k, l \notin \{i_1, i_2\}, x^k, x^l \not\preceq x^{i_1}, x^{i_2} \text{ and } y^{i_2}, y^l \not\preceq y^{i_1}, y^l\}| \\
&= \mathbf{1}_{(y^{i_2} \not\preceq y^{i_1})} \left( 2 \binom{n}{2} - |\{(k, l) : x^k \preceq x^{i_1} \text{ or } x^k \preceq x^{i_2} \text{ or } x^l \preceq x^{i_1} \text{ or } x^l \preceq x^{i_2} \right. \\
&\quad \left. \text{or } y^k \preceq y^l \text{ or } y^{i_2} \preceq y^l \text{ or } y^k \preceq y^{i_1}\}| \right). \tag{6.9}
\end{aligned}$$

Unlike in the prior derivations, the second to last term above has a condition which directly relates  $z^k$  and  $z^l$  and hence we cannot reduce to simple forms as in Equations (6.7), (6.8). Despite this, as we will now show, it is still possible to use orthogonal range queries to compute Equation (6.9). To see this, we construct a collection  $\mathcal{D}_{pair}$  of points in  $\mathbb{R}^{2d}$  consisting of the concatenation of all pairs  $z^i, z^j$  with  $i \neq j$ , that is we let

$$\mathcal{D}_{pair} = \{(z^i, z^j) = (x^i, y^i, x^j, y^j) \mid 1 \leq i \neq j \leq n\}.$$

$|\mathcal{D}_{pair}| = n(n-1)$  so that  $\mathcal{D}_{pair}$  takes  $O(n^2)$  time to construct. Since  $\mathcal{D}_{pair}$  contains  $n(n-1)$  elements of dimension  $2d$  we may construct an orthogonal range-tree on  $\mathcal{D}_{pair}$  in, recalling that we consider  $d$  to be bounded,  $O(n^2 \log_2(n^2)^{2d-1}) = O(n^2 \log_2(n)^{2d-1})$  time. Orthogonal range queries on  $\mathcal{D}_{pair}$  require  $O(\log_2(n)^{2d-1})$  time.

Let

$$\begin{aligned}
a_1 &= \{(k, l) \in B : x^k \preceq x^{i_1}\}, & a_2 &= \{(k, l) \in B : x^k \preceq x^{i_2}\}, \\
a_3 &= \{(k, l) \in B : x^l \preceq x^{i_1}\}, & a_4 &= \{(k, l) \in B : x^l \preceq x^{i_2}\}, \\
a_5 &= \{(k, l) \in B : y^k \preceq y^{i_1}\}, & a_6 &= \{(k, l) \in B : y^{i_2} \preceq y^l\}, \text{ and} \\
a_7 &= \{(k, l) \in B : y^k \preceq y^l\}
\end{aligned}$$

where  $B = \{(k, l) \in [n]^2 : k \neq l\}$ .

Using inclusion-exclusion we have that

$$\begin{aligned}
& 2 \binom{n}{2} - |\{(k, l) \in B : x^k \preceq x^{i_1} \text{ or } x^k \preceq x^{i_2} \text{ or } x^l \preceq x^{i_1} \text{ or } x^l \preceq x^{i_2} \\
& \quad \text{or } y^k \preceq y^l \text{ or } y^{i_2} \preceq y^l \text{ or } y^k \preceq y^{i_1}\}| \\
& = \sum_{L \subset [7]} (-1)^{|L|} |\cap_{i \in L} a_i| \\
& = \sum_{L \subset [6]} (-1)^{|L|} |\cap_{i \in L} a_i| + \sum_{L \subset [6]} (-1)^{|L|+1} |a_7 \cap (\cap_{i \in L} a_i)|
\end{aligned}$$

where we, in the above, let the empty intersection equal  $B$ . Now  $a_1, \dots, a_6$  are nothing more than orthogonal range constraints on elements in  $\mathcal{D}_{pair}$ , it follows that  $|\cap_{i \in L} a_i|$  for  $L \subset [6]$  can be computed by an orthogonal range query on  $\mathcal{D}_{pair}$ . Thus we can compute  $\sum_{L \subset [6]} (-1)^{|L|} |\cap_{i \in L} a_i|$  using  $2^6 = 64$  orthogonal range queries on  $\mathcal{D}_{pair}$  which takes  $O\{64 \log_2(n)^{2d-1}\} = O\{\log_2(n)^{2d-1}\}$  time.

It remains to show how we can compute  $\sum_{L \subset [6]} (-1)^{|L|} |a_7 \cap (\cap_{i \in L} a_i)|$ . Since  $a_7$  describes relationship between pairs  $y^k, y^l$  and thus is not a standard orthogonal range query constraint. Perhaps surprisingly, however, this does not pose a substantial obstacle. Consider the collection

$$\mathcal{D}_{pair}^* = \{(z^i, z^j) = (x^i, y^i, x^j, y^j) \mid 1 \leq i \neq j \leq n \text{ and } y^i \preceq y^j\},$$

$\mathcal{D}_{pair}^*$  is the subset of points in  $\mathcal{D}_{pair}$  which satisfy the condition in  $a_7$ . Clearly  $\mathcal{D}_{pair}^*$  can be constructed in  $O(n^2)$  time. Hence for any  $L \subset [6]$  we can compute  $a_7 \cap (\cap_{i \in L} a_i)$  by performing an orthogonal range query, with the constraints from  $\cap_{i \in L} a_i$ , on the set  $\mathcal{D}_{pair}^*$ . It follows that  $\sum_{L \subset [6]} (-1)^{|L|} |a_7 \cap (\cap_{i \in L} a_i)|$  can be computed with 64 orthogonal range queries, as with  $\mathcal{D}_{pair}$ , constructing a rangetree on  $\mathcal{D}_{pair}^*$  takes  $O\{n^2 \log_2(n)^{2d-1}\}$  and range query requires  $O\{\log_2(n)^{2d-1}\}$  time.

Finally, as  $U_{\tau_p^*}(z^{[n]})$  is a sum over  $n(n-1)$  choices for  $i_1, i_2$  and, for each  $i_1, i_2$ , we must compute (6.7), (6.8), and (6.9) which, from the above, requires  $O\{\log_2(n)^{2d-1}\}$  time. Hence assuming the range-trees on  $\mathcal{D}_{pair}$  and  $\mathcal{D}_{pair}^*$  have already been constructed, computing

$U_{\tau_P^*}(z^{[n]})$  requires  $O\{n(n-1)\log_2(n)^{2d-1}\} = O\{n^2\log_2(n)^{2d-1}\}$  time. As constructing the range-trees on  $\mathcal{D}_{pair}$  and  $\mathcal{D}_{pair}^*$  require each  $O\{n^2\log_2(n)^{2d-1}\}$  time it follows that the total asymptotic computation time of  $U_{\tau_P^*}(z^{[n]})$  is  $O\{n^2\log_2(n)^{2d-1}\}$ .

A similar argument shows that  $U_{\tau_J^*}$  can also be computed in  $O\{n^2\log_2(n)^{2d-1}\}$  time.

### 6.5 Empirical Computational Efficiency

Here we empirically compare the computational complexity of computing  $U_D, U_R, U_{\tau_J^*}$ , and  $U_{\tau_P^*}$ . For these simulations we will generate data from two different distributions; for the first, we let  $(X, Y) \sim N_2(0, I_2)$  while, for the second, we let  $(X, Y) = (X^1, X^2, Y) \sim N_3(0, I_3)$ . We consider the following experiments.

We compute  $U_D$  using Equation (6.5) where counts are either computed with a range-tree or looping through the data set. The asymptotic run-time of the range-tree method is  $O\{n\log_2(n)^{d-1}\}$  with the more naïve method taking  $O(n^2)$  time. Both of the above methods are substantially faster than the  $O(n^5)$  strategy of directly computing the sum in Equation (6.2).

We compute  $U_R$  using Equation (6.6) where counts are either computed with an orthogonal range tensor or by looping through the data set. The asymptotic run-time of the orthogonal range tensor method is  $O(n^d)$  while the naïve method takes  $O(n^{d+1})$  time. As above, both of these methods are much faster than the truly naïve  $O(n^{d+4})$  strategy.

We compute both  $U_{\tau_J^*}$  and  $U_{\tau_P^*}$  using our range-tree methods and by definition. The range-tree methods require  $O\{n^2\log_2(n)^{2d-1}\}$  time while the naïve methods take  $O(n^4)$  time.

The results of the above computations are shown in Figure 6.5.1. From the asymptotic analysis, one would expect that the benefits of using our efficient range query data structures would diminish in higher dimensions and, indeed, that is exactly what the figures show. Comparing Figures 6.5.1a and 6.5.1b, for instance, we see that when  $(X, Y) \sim N_2(0, I_2)$  the naïve algorithm performs worse than the other for almost all sample sizes but, when moving up to dimension 3 with  $(X, Y) \sim N_3(0, I_3)$ , it is only for sample sizes greater than  $\sim 3000$  that the range-tree method out-performs the naïve strategy.

As Figure 6.5.1f shows, computing  $U_{\tau_p^*}$  using range-trees is, for reasonable sample sizes, substantially slower than computing  $U_{\tau_p^*}$  by definition. This is not surprising considering the many large constant factors that are hidden in the asymptotic analysis.

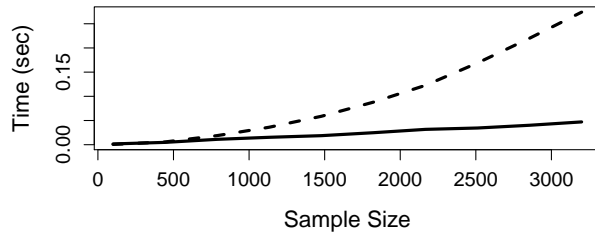
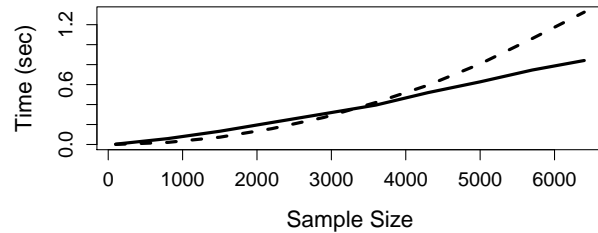
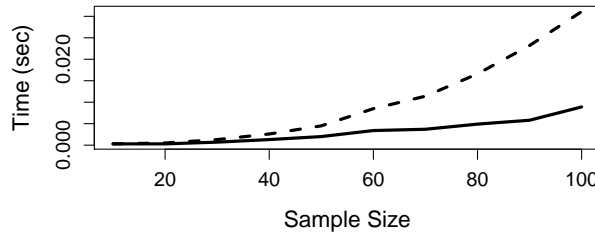
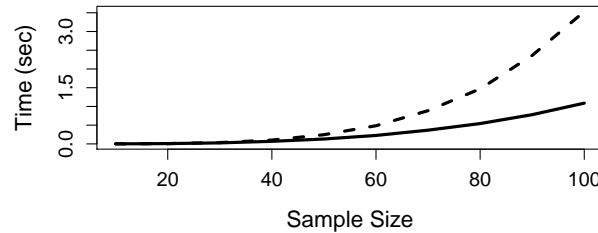
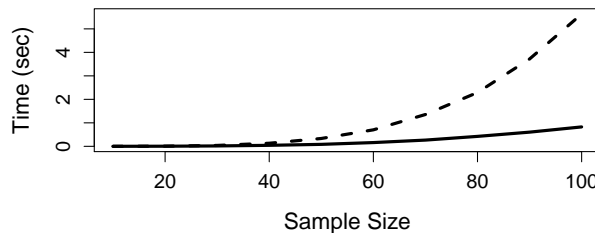
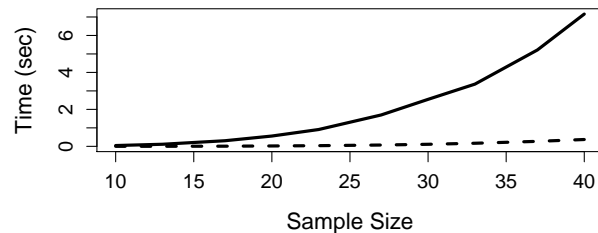
(a)  $U_D, (X, Y) \sim N_2(0, I_2)$ (b)  $U_D, (X, Y) \sim N_3(0, I_3)$ (c)  $U_R, (X, Y) \sim N_2(0, I_2)$ (d)  $U_R, (X, Y) \sim N_3(0, I_3)$ (e)  $U_{\tau_j^*}, (X, Y) \sim N_3(0, I_3)$ (f)  $U_{\tau_P^*}, (X, Y) \sim N_3(0, I_3)$ 

Figure 6.5.1: The computation time of our U-statistics at various sample sizes comparing the benefits of using (solid lines), and not using (dashed lines), efficient data structures for orthogonal range queries. The naïve methods are substantially slower except for two cases, for sample sizes less than  $\approx 3000$  in (b) and for all tested sample sizes in (f).

## Chapter 7

**LARGE SAMPLE THEORY**

In this chapter we consider the asymptotic properties of U-statistics estimating symmetric rank covariances. After a review of the asymptotic theory of U-statistics we will develop general conditions which guarantee that the U-statistic estimating a symmetric rank covariance has a non-Gaussian asymptotic distribution under the null hypothesis of independence. In the bivariate setting, these results will allow us to derive explicit, computable, asymptotic distributions for  $U_{\tau^*}$  under the null hypothesis of independence when  $X$  and  $Y$  are drawn from continuous or discrete distributions. Moreover, in this bivariate case, we will be able to show that the asymptotic distributions of the U-statistics corresponding to  $D$ ,  $R$ , and  $\tau^*$  are, up to scaling, equal when  $X$  and  $Y$  are continuous and independent.

**7.1 Asymptotic Theory of U-statistics**

This section gives a brief review of the asymptotic theory of U-statistics we require, the book of Serfling (1980) provides an in-depth introduction to the topic for the interested reader. Let  $Z^1, Z^2, \dots$  be independent and identically distributed random vectors taking their values in  $\mathbb{R}^d$  with  $d \geq 1$ . We say a function  $\kappa : \mathbb{R}^{d \times m} \rightarrow \mathbb{R}$  is a *symmetric kernel function* if its value is invariant to any permutation of its  $m$  arguments. Given a symmetric kernel function  $\kappa$ , we call

$$U_n = \frac{1}{\binom{n}{m}} \sum_{(i_1, \dots, i_m) \in C(n, m)} \kappa(Z_{i_1}, \dots, Z_{i_m}), \quad (7.1)$$

the U-statistic with kernel  $\kappa$ . Here,  $C(n, m) = \{(i_1, \dots, i_m) \in \{1, \dots, n\}^m : i_1 < i_2 < \dots < i_m\}$ . Clearly,  $\theta := E\kappa(Z^1, \dots, Z^m) = EU_n$ .

The asymptotics of U-statistics rely deeply on the functions

$$\kappa_i(z_1, \dots, z_i) = E\{\kappa(z_1, \dots, z_i, Z_{i+1}, \dots, Z_m)\}, \quad (i = 1, \dots, m), \quad (7.2)$$

and their variances

$$\sigma_i^2 = \text{Var}\{\kappa_i(Z_1, \dots, Z_i)\}, \quad (i = 1, \dots, m). \quad (7.3)$$

It is well known that  $\sigma_1^2 \leq \sigma_2^2 \leq \dots \leq \sigma_m^2$ .

**Theorem 7.1** (Serfling (1980)). *If the kernel  $\kappa$  of the statistic  $U_n$  from (7.1) has variance  $\sigma_m^2 < \infty$ , then*

$$n^{1/2}(U_n - \theta) \rightarrow N(0, m^2\sigma_1^2)$$

*in distribution.*

If  $\sigma_1^2 = 0$  then the above asymptotic Gaussian distribution is degenerate and  $n^{1/2}(U_n - \theta) \rightarrow 0$  in probability. If  $\sigma_1^2 = 0$  and  $\sigma_2^2 > 0$ , then  $U_n$  is a degenerate of order two and one obtains a non-degenerate limiting distribution by scaling  $U_n$  by a factor of  $n$ . In this case, the limiting distribution is determined by the eigenvalues of the operator  $A_\kappa$  which maps a square integrable function  $g : \mathbb{R}^d \rightarrow \mathbb{R}$  to the function  $z \mapsto E[\{\kappa_2(z, Z_1) - \theta\}g(Z_1)]$ .

**Theorem 7.2** (Serfling (1980)). *If the kernel  $\kappa$  of the statistic  $U_n$  from (7.1) has variance  $\sigma_m^2 < \infty$  and  $\sigma_1^2 = 0 < \sigma_2^2$ , then*

$$n(U_n - \theta) \rightarrow \binom{m}{2} \sum_{i=1}^{\infty} \lambda_i (\chi_{1i}^2 - 1)$$

*in distribution where  $\chi_{11}^2, \chi_{12}^2, \dots$  are independent and identically distributed random variables that follow a chi-square distribution with 1 degree of freedom, and the  $\lambda_i$ 's are the eigenvalues, taken with multiplicity, associated with a system of orthonormal eigenfunctions of the operator  $A_\kappa$ .*

## 7.2 Null Asymptotics

Let  $\mu$  be a symmetric rank covariance and let  $k$  and  $\kappa$  be the unsymmetrized and symmetrized kernel functions corresponding to  $\mu$  as in Chapter 6. From Section 7.1 we saw that determining the asymptotic distribution of  $U_\mu$  under the null hypothesis of independence, that  $X \perp\!\!\!\perp Y$ , requires an understanding of the functions

$$\kappa_i(z^1, \dots, z^i) = E\{\kappa(z^1, \dots, z^i, Z^{i+1}, \dots, Z^m)\}.$$

To this end, we introduce some simplifying lemmas and propositions.

**Lemma 7.3.** *Suppose that  $X \perp\!\!\!\perp Y$ . Let  $S \subset [m]$  and let  $G$  be the invariance group corresponding to  $\mu$ . Partition  $H$  into equivalence classes  $E_1, \dots, E_t$  where  $h, h' \in H$  are equivalent if there exists  $g \in G$  such that  $gh(i) = h'(i)$  for all  $i \in S$ . If each  $E_i$  contains an equal number of even and odd permutations then for any  $z_1, \dots, z_m \in \mathbb{R}^{r+s}$ ,  $E\{k(W^{[m]})\} = 0$  where  $W^i = z^i$  if  $i \in S$  and  $W^i = Z^i$  otherwise.*

Lemma 7.3 allows us to identify conditions guaranteeing that  $U_\mu$  is degenerate, that is, cases in which  $n^{1/2}(U_\mu - EU_\mu)$  converges to 0 in probability.

**Proposition 7.4.** *Suppose that the conditions of Lemma 7.3 hold for  $\mu$  whenever  $S$  is a singleton set. If  $X \perp\!\!\!\perp Y$  then  $\kappa_1 \equiv 0$  and thus  $U_\mu$  is a degenerate  $U$ -statistic.*

As an application of Lemma 7.3 and Proposition 7.4 we show the known result that  $\tau^*$ ,  $D$ , and  $R$  are degenerate  $U$ -statistics under independence, and, additionally, that their  $\kappa_2$  functions take a simple form.

**Lemma 7.5.** *Let  $I_X, I_Y$  be rank indicators of order  $m \geq 4$  and dimensions  $r$  and  $s$  respectively. Let  $\mu = \mu_{I_X, I_Y, H_{\tau^*}}$  be a symmetric rank covariance. Suppose that  $X \perp\!\!\!\perp Y$ . If the invariance group of  $\mu$  contains the subgroup  $G = \langle (1\ 2), (3\ 4) \rangle$ , then  $\kappa_1(z^1) \equiv 0$ , so  $U_\mu$  is a degenerate  $U$ -statistic and*

$$\kappa_2(z^1, z^2) = \frac{4}{\binom{m}{2}} E\left\{a_{I_X}(x^1, x^2, X^{3, \dots, m})\right\} E\left\{a_{I_Y}(y^1, y^2, Y^{3, \dots, m})\right\}$$

where for any rank indicator  $I$  of order  $m \geq 4$  we define

$$a_I(w^{[m]}) = \sum_{\sigma \in H_{\tau^*}} \text{sign}(\sigma) I(w^{\sigma^{[m]}}).$$

By construction, all multivariate  $\tau^*$  extensions satisfy the above conditions, as do  $\tau^*$ ,  $D$ , and  $R$ .

In the next section we will use the above lemma to clarify the exact large sample behavior of  $U_{\tau^*}$  in the case where both  $X$  and  $Y$  are univariate and independent. As a corollary this will also allow us to show that  $U_{\tau^*}$ ,  $U_D$ , and  $U_R$  have, up to a scale multiple, the same asymptotic distribution under the null hypothesis that  $X \perp\!\!\!\perp Y$  and  $(X, Y)$  are drawn from a continuous bivariate distribution. The general case, where  $X$  and  $Y$  may be multivariate, appears to be significantly more difficult. In part this is because, unlike in the continuous bivariate case, the distributions of the random vectors  $X$  and  $Y$  influence the asymptotic properties of our multivariate U-statistics. Indeed, even when  $r = 1$  and  $s = 2$  and  $X, Y$  are normally distributed, Figure 7.2.1 suggests that the correlation between  $Y_1$  and  $Y_2$  impacts the large sample behavior. Because of these difficulties, we leave this multivariate case for future work.

### 7.3 Explicit Large-Sample Behavior in the Bivariate Case

For this section we will let  $r = s = 1$  and focus on the U-statistic

$$U_{\tau^*}(z^{[n]}) = \frac{1}{\binom{n}{4}} \sum_{1 \leq i_1 < \dots < i_4 \leq n} \kappa^{\tau^*}(z^{i_1, \dots, i_4})$$

where for  $w^4 \in \mathbb{R}^{4 \times 1}$  we have

$$\begin{aligned} \kappa^{\tau^*}(z^{[4]}) &= \frac{1}{24} \sum_{\sigma \in S_4} k^{\tau^*}(z^{\sigma^{[4]}}), & k^{\tau^*}(z^{[4]}) &= a(x^{[4]})a(y^{[4]}), \\ a_{I_{\tau^*}}(w^{[4]}) &= \sum_{\sigma \in H_{\tau^*}} \text{sign}(\sigma) I_{\tau^*}(w^{\sigma^{[4]}}), & I_{\tau^*}(w^{[4]}) &= 1_{(w^1, w^2 < w^3, w^4)}. \end{aligned}$$

Now, by Lemma 7.5 we have that, under the null hypothesis that  $X \perp\!\!\!\perp Y$ ,

$$\kappa_2^{\tau^*}(z^1, z^2) = \frac{2}{3} E\{a_{I_{\tau^*}}(x^1, x^2, X^3, X^4)\} E\{a_{I_{\tau^*}}(y^1, y^2, Y^3, Y^4)\}. \quad (7.4)$$

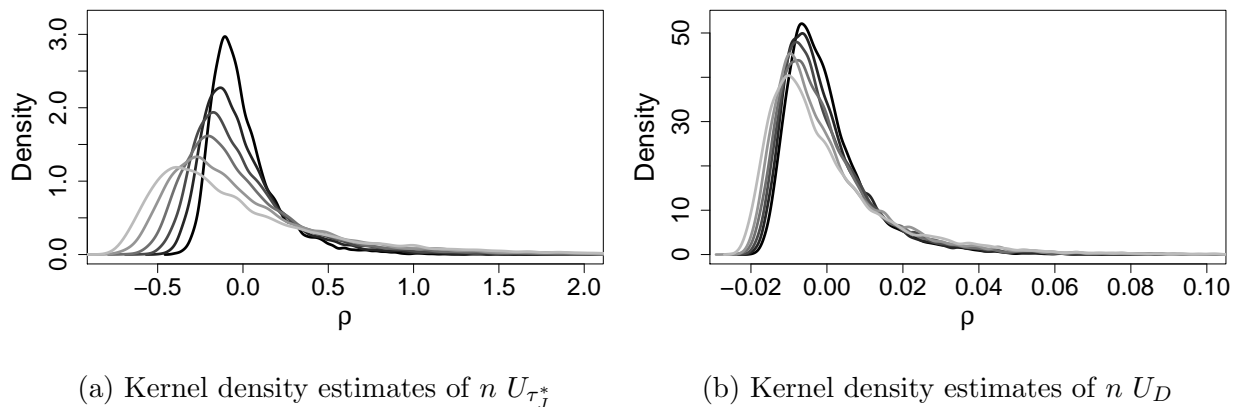


Figure 7.2.1: Kernel density estimates of the finite sample distributions of  $n U_{\tau_j^*}$  and  $n U_D$  for samples of size  $n = 70$  taken from  $(X, Y)$  where  $X, Y_1, Y_2 \sim N(0, 1)$ ,  $(Y_1, Y_2)$  are jointly normal with correlation  $\rho$ , and  $X \perp Y$ . Here  $\rho$  varies in  $\{0, 1/5, \dots, 1\}$  with the lighter colored lines corresponding to kernel density estimates for smaller  $\rho$ .

In the following we will clarify the large sample behavior of  $U_{\tau^*}$  under the null hypothesis of independence by finding an explicit representation for  $\kappa_2^*$  and using this representation to compute the eigenvalues of the operator  $A_{\kappa^{\tau^*}}$  which maps a square integrable function  $g : \mathbb{R}^2 \rightarrow \mathbb{R}$  to the function  $z \mapsto E[\kappa_2(z, Z_1)g(Z_1)]$ , recall Theorem 7.2. We will do this under three cases corresponding to distributional assumptions on  $X$  and  $Y$ . Code for performing asymptotic tests of independence using the results of the following sections can be found in the open source package `TauStar`<sup>1</sup> R available on CRAN, the Comprehensive R Archive Network (R Core Team, 2018; Weihs, 2015). Before moving to our main results, the following lemma will be useful in computing the eigenvalues of the operator  $A_{\kappa^{\tau^*}}$ .

**Lemma 7.6.** *Let  $g_1, g_2 : \mathbb{R}^2 \rightarrow \mathbb{R}$  be symmetric real-valued functions with  $E\{g_1(X_1, X_2)\} = E\{g_2(Y_1, Y_2)\} = 0$  and  $E\{g_1(X_1, X_2)^2\}, E\{g_2(Y_1, Y_2)^2\} < \infty$  For  $i = 1, 2$ , let  $\lambda_{i,j}$ ,  $j \in \mathbb{N}_+$ , be the nonzero eigenvalues of  $A_{g_i}$  taken with multiplicity. Then the products  $\lambda_{1,j_1} \lambda_{2,j_2}$ ,  $j_1, j_2 \in$*

<sup>1</sup>See <https://cran.r-project.org/web/packages/TauStar/index.html>

$\mathbb{N}_+$ , are the nonzero eigenvalues of  $A_k$ , again taken with multiplicity, for  $k((x_1, y_1), (x_2, y_2)) := g_1(x_1, x_2)g_2(y_1, y_2)$ .

### 7.3.1 The jointly continuous case

Suppose now that  $X \perp\!\!\!\perp Y$  with  $X$  and  $Y$  following continuous marginal distributions. Since  $\tau^*$  (and  $U_{\tau^*}$ ) are nonparametric, they are invariant to monotonically increasing transformations of the marginals of  $(X, Y)$ . As such we may, and will, assume that  $X$  and  $Y$  are i.i.d.  $\text{Uniform}(0, 1)$ . Then  $(X, Y)$  is uniform on the unit square  $(0, 1) \times (0, 1)$ . In this case  $\kappa_2^{\tau^*}$  has a particularly nice form.

**Lemma 7.7.** *If  $X, Y \stackrel{i.i.d.}{\sim} \text{Uniform}(0, 1)$ , then for  $z_1, z_2 \in (0, 1)^2$ ,*

$$\kappa_2^{\tau^*}(z^{[2]}) = 6c(x_1, x_2)c(y_1, y_2)$$

where

$$c(x_1, x_2) = \frac{1}{2}x_1^2 + \frac{1}{2}x_2^2 - x_1 \vee x_2 + \frac{1}{3}$$

and  $x_1 \vee x_2 := \max\{x_1, x_2\}$ .

Somewhat surprisingly, the function  $c$  corresponds to the kernel of the well studied Cramér-von Mises statistic. Leveraging that the eigenvalues of  $A_c$  are already known, we are now able to derive the asymptotic distribution of  $t^*$ .

**Theorem 7.8.** *If  $X$  and  $Y$  are independent continuous random variables, then*

$$nU_{\tau^*} \xrightarrow{d} T := \frac{36}{\pi^4} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{1}{i^2 j^2} (\chi_{1,ij}^2 - 1) \quad (7.5)$$

where  $\{\chi_{1,ij}^2 : i, j \in \mathbb{N}_+\}$  is a collection of i.i.d.  $\chi_1^2$  random variables.

Remarkably as the next theorem shows, the asymptotic distributions of  $U_D$  and  $U_R$  are scale multiples of  $T$ .

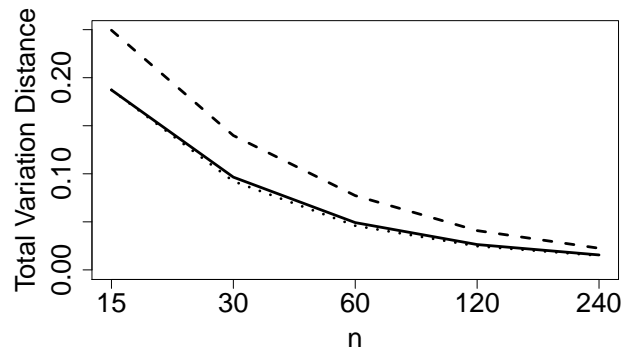


Figure 7.3.2: The total variation distance from kernel density estimators of the finite sample distributions of  $U_{\tau^*}$  (solid line),  $U_D$  (dashed line), and  $U_R$  (dotted line) to the probability density functions of their asymptotic distributions. The x-axis is plotted on a log-scale. Here  $n \in \{15, 30, 60, 120, 240\}$  is the sample size. The finite sample distributions are quite close to the asymptotic distributions even when  $n$  is only  $\approx 60$ .

**Proposition 7.9.** *Suppose we are in the setting of Theorem 7.8. Then both  $nU_D$ ,  $nU_R \rightarrow T/36$  in distribution.*

To better understand at which sample size  $n$  the finite-sample distributions of  $U_{\tau^*}$ ,  $U_D$ , and  $U_R$  become well-approximated by their asymptotic distributions, Figure 7.3.2 shows the total variation distance between kernel density estimates of the finite sample distributions of  $U_{\tau^*}$ ,  $U_D$ , and  $U_R$  for  $n \in \{15, 30, 60, 120, 240\}$  against the probability density functions of their asymptotic distributions. We observe good agreement even for  $n = 60$ .

### 7.3.2 Discrete variables

We now treat the case where  $X$  and  $Y$  are independent discrete random variables with finite supports. Unlike in the continuous case, the asymptotic distribution of  $U_{\tau^*}$  now depends on how  $X$  and  $Y$  distribute their probability mass marginally. In practical applications these marginal probabilities must be estimated before using our limit theorem.

In order to present the result, we associate a matrix to a discrete random variable as

follows. Let  $U$  be a random variable with finite support  $\{u_1, \dots, u_a\}$ , cumulative distribution function  $F$ , and probability mass function  $p$ . We then define  $R^U$  to be the  $a \times a$  symmetric matrix whose  $(i, j)$ -th entry is

$$R_{ij}^U = \sqrt{p(u_i)p(u_j)} \left\{ \left[ (F(u_i \wedge u_j) - p(u_i \wedge u_j))^2 + (1 - F(u_i \vee u_j))^2 \right] - \right. \quad (7.6)$$

$$\left. I(u_i \neq u_j) \left[ F(u_i \wedge u_j)(1 - F(u_i \wedge u_j)) + \sum_{u_i \wedge u_j < u_\ell < u_i \vee u_j} p(u_\ell)(1 - F(u_\ell)) \right] \right\}.$$

**Theorem 7.10.** *Let  $X$  and  $Y$  be independent discrete random variables with finite supports of size  $a$  and  $b$ , respectively. Let  $\lambda_1^X, \dots, \lambda_a^X$  be the eigenvalues of  $R^X$ , and let  $\lambda_1^Y, \dots, \lambda_b^Y$  be the eigenvalues of  $R^Y$ . Then*

$$nU_{\tau^*} \xrightarrow{d} 4 \sum_{i=1}^a \sum_{j=1}^b \lambda_i^X \lambda_j^Y (\chi_{1,ij}^2 - 1)$$

where  $\{\chi_{1,ij}^2 : i \leq r, j \leq s\}$  is a collection of  $rs$  i.i.d.  $\chi_1^2$  random variables.

In the special case that  $X$  and  $Y$  are Bernoulli random variables, the asymptotic distribution can be presented in simple form.

**Example 7.11.** If  $X \sim \text{Bernoulli}(p)$  for  $p \in (0, 1)$ , then

$$R^X = \begin{pmatrix} p^2(1-p) & -(p(1-p))^{3/2} \\ -(p(1-p))^{3/2} & p(1-p)^2 \end{pmatrix}$$

has rank one and its nonzero eigenvalue is  $p(1-p)$ . It follows that if  $Y$  is a second independent random variable with  $Y \sim \text{Bernoulli}(q)$  for  $q \in (0, 1)$ , then

$$nU_{\tau^*} \xrightarrow{d} 4pq(1-p)(1-q)(\chi_1^2 - 1).$$

So,  $U_{\tau^*}$  can be centered and scaled to become asymptotically chi-square.

**Example 7.12.** For a ternary random variable  $X$  with  $P(X = 1) = p_1$ ,  $P(X = 2) = p_2$  and  $P(X = 3) = p_3 = 1 - p_1 - p_2$ , we have

$$R^X = \begin{pmatrix} p_1(1-p_1)^2 & -\sqrt{p_1 p_2} [p_1(1-p_1) - p_3^2] & -\sqrt{p_1 p_3} [p_3(1-p_3) + p_1 p_2] \\ \cdot & p_2(p_1^2 + p_3^2) & -\sqrt{p_2 p_3} [p_3(1-p_3) - p_1^2] \\ \cdot & \cdot & p_3(1-p_3)^2 \end{pmatrix},$$

where we show only the upper half of the symmetric matrix. No simple formula seems to be available to determine the eigenvalues of  $R^X$  in this case, but the eigenvalues can readily be computed numerically for any (possibly estimated) values of  $p_1$  and  $p_2$ .

Finally, if  $X$  is discrete with finite support and  $Y$  is continuous, then a simple extension of Theorems 7.8 and 7.10 gives the following result.

**Corollary 7.13.** *Let  $X$  and  $Y$  be independent random variables, where  $X$  has finite support of size  $r$  and  $Y$  is continuous. Let  $\lambda_1, \dots, \lambda_r$  be the eigenvalues of  $R^X$ . Then*

$$nU_{\tau^*} \xrightarrow{d} \frac{12}{\pi^2} \sum_{i=1}^r \sum_{j=1}^{\infty} \frac{\lambda_i}{j^2} (\chi_{1,ij}^2 - 1)$$

where  $\{\chi_{1,ij}^2 : i \leq r, j \in \mathbb{N}_+\}$  is a collection of i.i.d.  $\chi_1^2$  random variables.

## Appendix B

### PROOFS FOR PART II

#### B.1 Proofs for Chapter 4

##### PROOF OF THEOREM 4.11

If  $X \perp\!\!\!\perp Y$ , then  $R(X, Y) = 0$  because  $F_{XY} = F_X F_Y$ .

Now suppose that  $X \not\perp\!\!\!\perp Y$ . Then, by the definition of independence, there exist  $(x, y) \in \mathbb{R}^{r+s}$  such that  $F_{XY}(x, y) \neq F_X(x)F_Y(y)$ . Since  $F_{XY}(x, y) \leq \min\{F_X(x), F_Y(y)\}$ ,  $F_{XY}(x, y) \neq F_X(x)F_Y(y)$  implies that  $F_X(x), F_Y(y) > 0$ .

We now define  $\tilde{x} \in \mathbb{R}^r, \tilde{y} \in \mathbb{R}^s$  as follows. Let

$$\begin{aligned}\tilde{x}_i &= \arg \min\{x^* \mid x^* \leq x_i \text{ and } F_{X_i}(x^*) = F_{X_i}(x_i)\} \quad (i = 1, \dots, r) \\ \tilde{y}_i &= \arg \min\{y^* \mid y^* \leq y_i \text{ and } F_{Y_i}(y^*) = F_{Y_i}(y_i)\} \quad (i = 1, \dots, s).\end{aligned}$$

By the right continuity of cumulative distribution functions, we have that such  $\tilde{x}_i, \tilde{y}_i$  exist and that  $F_{X_i}(\tilde{x}_i) = F_{X_i}(x_i)$  and  $F_{Y_j}(\tilde{y}_j) = F_{Y_j}(y_j)$  for all  $i$  and  $j$ . We will now show that  $F_{XY}(\tilde{x}, \tilde{y}) = F_{X,Y}(x, y)$ . Clearly  $F_{XY}(\tilde{x}, \tilde{y}) \leq F_{X,Y}(x, y)$ . Suppose, for contradiction, that  $F_{XY}(\tilde{x}, \tilde{y}) < F_{X,Y}(x, y)$ . Write  $\tilde{z} = (\tilde{x}, \tilde{y})$  and let  $i$  be the smallest index for which  $F_{XY}(\tilde{z}_1, \dots, \tilde{z}_i, z_{i+1}, \dots, z_{r+s}) < F_{X,Y}(z)$ , by assumption such an  $i$  exists. Without loss of generality assume that  $i \leq r$ . Then we have that

$$\begin{aligned}F_{X_i}(x_i) &= P(X_i \leq x_i) \\ &= F_{XY}(\tilde{x}_1, \dots, \tilde{x}_{i-1}, x_i, x_{i+1}, \dots, x_r, y) + P\{X_i \leq x_i \text{ and } (X_1 > \tilde{x}_1 \text{ or } \dots \text{ or } Y_s > y_s)\}.\end{aligned}$$

Now clearly both  $F_{XY}(\tilde{x}_1, \dots, \tilde{x}_{i-1}, x_i, x_{i+1}, \dots, x_r)$  and  $P\{X_i \leq x_i \text{ and } (X_1 > \tilde{x}_1 \text{ or } \dots \text{ or } Y_s > y_s)\}$  are non-decreasing in  $x_i$  and thus, since  $F_{XY}(\tilde{z}_1, \dots, \tilde{z}_i, z_{i+1}, \dots, z_{r+s}) < F_{X,Y}(z)$ , we

have that

$$\begin{aligned} F_{X_i}(x_i) &> F_{XY}(\tilde{x}_1, \dots, \tilde{x}_{i-1}, \tilde{x}_i, x_{i+1}, \dots, x_r) + P\{X_i \leq \tilde{x}_i \text{ and } (X_1 > \tilde{x}_1 \text{ or } \dots \text{ or } Y_s > y_s)\} \\ &= F_{X_i}(\tilde{x}_i). \end{aligned}$$

But this contradicts what we have shown above, that  $F_{X_i}(x_i) = F_{X_i}(\tilde{x}_i)$ . It follows that  $F_{XY}(\tilde{x}, \tilde{y}) = F_{XY}(x, y)$  as claimed. An essentially identical argument to the one above also shows that  $F_X(\tilde{x}) = F_X(x)$  and  $F_Y(\tilde{y}) = F_Y(y)$ . Hence we have that

$$F_{XY}(\tilde{x}, \tilde{y}) - F_X(\tilde{x})F_Y(\tilde{y}) = F_{XY}(x, y) - F_X(x)F_Y(y) \neq 0.$$

Now let  $\mathcal{I}_X = \{i \in [r] \mid \lim_{x^* \rightarrow \tilde{x}_i^-} F_{X_i}(x^*) \neq F_{X_i}(\tilde{x}_i)\}$  so that for all  $i \in \mathcal{I}_X$  we have that  $F_{X_i}$  has a jump discontinuity at  $\tilde{x}_i$  and thus  $P(X_i = \tilde{x}_i) > 0$ . Let  $\mathcal{I}_Y$  be the corresponding set of such indices for the  $F_{Y_i}$ . Now, for any  $i \in [r]$  and  $\delta > 0$  define  $B_\delta^i = [\tilde{x}_i - \delta, \tilde{x}_i]$  if  $i \notin \mathcal{I}_X$  and  $B_\delta^i = \{\tilde{x}_i\}$  if  $i \in \mathcal{I}_X$ . By our definition of  $\tilde{x}_i$  and  $\mathcal{I}_X$  we have that  $P(X_i \in B_\delta^i) > 0$ . Similarly define, for any  $i \in [s]$  and  $\delta > 0$ ,  $C_\delta^i = [\tilde{y}_i - \delta, \tilde{y}_i]$  if  $i \notin \mathcal{I}_Y$  and  $C_\delta^i = \{\tilde{y}_i\}$  if otherwise. Again we have that  $P(Y_i \in C_\delta^i) > 0$ . Let  $B_\delta = B_\delta^1 \times \dots \times B_\delta^r$  and  $C_\delta = C_\delta^1 \times \dots \times C_\delta^s$ .

Claim: there exists  $\delta > 0$  such that for all

$$(x, y) \in D_\delta = B_\delta \times C_\delta$$

we have  $F_{XY}(x, y) - F_X(x)F_Y(y) \neq 0$ .

If this claim is true we have that

$$\begin{aligned} R(X, Y) &= \int_{\mathbb{R}^{r+s}} \{F_{XY}(x, y) - F_X(x)F_Y(y)\}^2 \prod_{i=1}^r dF_{X_i}(x_i) \prod_{j=1}^s dF_{Y_j}(y_j) \\ &\geq \int_{D_\delta} \{F_{XY}(x, y) - F_X(x)F_Y(y)\}^2 \prod_{i=1}^r dF_{X_i}(x_i) \prod_{j=1}^s dF_{Y_j}(y_j) \\ &> 0 \end{aligned}$$

where the last inequality follows since  $D_\delta$  has positive measure under  $dF_{X_i}(x_i) \prod_{j=1}^s dF_{Y_j}(y_j)$  and  $\{F_{XY}(x, y) - F_X(x)F_Y(y)\}^2$  is strictly positive for  $(x, y) \in D_\delta$ .

We now prove the claim. First let  $\varphi : [0, \infty] \rightarrow \mathbb{R}^r$  be defined such that, for all  $t \in [0, \infty]$ ,  $\varphi(t)_i = \tilde{x}_i$  if  $i \in \mathcal{I}_X$  and  $\varphi(t)_i = t\tilde{x}_i$  if  $i \notin \mathcal{I}_X$ . Each  $\varphi(t)_i$  is non-decreasing in  $t$ . Next consider the function  $G : [0, \infty] \rightarrow [0, 1]$  defined such that  $G(t) = F_X\{\varphi(t)\}$ .  $G$  is monotone non-decreasing and so has only jump discontinuities. If  $G$  does not have a jump discontinuity at  $t = 1$  then for any  $\epsilon > 0$  we may pick  $\delta < 1$  sufficiently small that

$$F_X(\tilde{x}) - F_X\{\varphi(s)\} = |F_X(\tilde{x}) - F_X\{\varphi(s)\}| = |G(1) - G(s)| < \epsilon$$

for all  $1 - \delta \leq s \leq 1$ . But for any  $x \in B_\delta$  we have  $\varphi(1 - \delta) \preceq x \preceq \tilde{x}$  and thus

$$|F_X(\tilde{x}) - F_X(x)| = F_X(\tilde{x}) - F_X(x) = F_X(\tilde{x}) - F_X(\{1 - \delta\}\tilde{x}) = G(1) - G(1 - \delta) < \epsilon.$$

Now suppose otherwise that  $G(t)$  has a jump discontinuity at  $t = 1$ . That is, we have  $F_X(\tilde{x}) - \lim_{t \rightarrow 1^-} G(t) = a > 0$ . Then, by the monotone convergence theorem,

$$\begin{aligned} a &= F_X(\tilde{x}) - \lim_{t \rightarrow 1^-} G(t) \\ &= P\left(\bigwedge_{i=1}^r X_i \leq \tilde{x}_i\right) - P\left\{\bigwedge_{i \in \mathcal{I}_X} (X_i \leq \tilde{x}_i) \wedge \bigwedge_{i \notin \mathcal{I}_X} (X_i < \tilde{x}_i)\right\} \\ &= P\left\{\bigwedge_{i \in \mathcal{I}_X} (X_i \leq \tilde{x}_i) \wedge \bigvee_{i \notin \mathcal{I}_X} (X_i = \tilde{x}_i)\right\} \\ &\leq P\left(\bigvee_{i \notin \mathcal{I}_X} X_i = \tilde{x}_i\right) \\ &\leq \sum_{i \notin \mathcal{I}_X} P(X_i = \tilde{x}_i). \end{aligned}$$

But by definition of  $\mathcal{I}_X$  we have that  $P(X_i = \tilde{x}_i) = 0$  for all  $i \in \mathcal{I}_X$ , it thus follows that  $0 < a \leq 0$  a contradiction. Hence  $G(t)$  does not have a jump discontinuity at  $t = 1$ .

Similar arguments hold for  $F_Y$  and  $F_{XY}$  and hence, for any  $\epsilon > 0$  there exists some  $\delta > 0$  such that for any  $(x, y) \in B_\delta \times C_\delta$  we have  $|F(\tilde{x}, \tilde{y}) - F_{XY}(x, y)|, |F(\tilde{x}) - F_X(x)|, |F(\tilde{y}) - F_Y(y)| < \epsilon$ . Thus, choosing  $\epsilon > 0$  sufficient small, clearly there exists  $\delta$  such that  $F_{XY}(x, y) - F_X(x)F_Y(y) \neq 0$  for all  $(x, y) \in B_\delta \times C_\delta$ . This completes the proof as noted above.  $\square$

## B.2 Proofs for Chapter 5

### B.2.1 Proofs for Section 5.1

#### PROOF OF PROPOSITION 5.6

Bergsma and Dassios (2014) show that

$$\tau^* = E\{a(X^{[4]}) a(Y^{[4]})\}$$

where

$$a(w^{[4]}) = 1_{(w^1, w^2 < w^3, w^4)} + 1_{(w^3, w^4 < w^1, w^2)} - 1_{(w^1, w^3 < w^2, w^4)} - 1_{(w^2, w^4 < w^1, w^3)}.$$

This is exactly our claimed result.

Recall that  $\tau$  can be expressed as

$$\tau = E[2 1_{(X^1 < X^2)} \{1_{(Y^1 < Y^2)} - 1_{(Y^2 < Y^1)}\}].$$

Lemma 5.11 then immediately gives our result for  $\tau$ . Moreover, letting  $\gamma = \nu = \tau$  in the proof of Proposition 5.9 and relabeling 2 as 4, and vice versa, we have our claimed form for  $\tau^2$ .

We now show that our result for  $D$ . For any  $z = (x, y) \in \mathbb{R}^{r+s}$  let, omitting subscripts on  $F_{XY}, F_X, F_Y$  for space,

$$c^+(x, y) = F(x, y)^2 \{1 - F(x) - F(y) + F(x, y)\}^2, \quad (\text{B.1})$$

$$c^-(x, y) = \{F(x) - F(x, y)\}^2 \{F(y) - F(x, y)\}^2, \quad (\text{B.2})$$

$$c(x, y) = c^+(x, y) + c^-(x, y), \quad (\text{B.3})$$

$$d(x, y) = \{c^+(x, y)c^-(x, y)\}^{1/2} \quad (\text{B.4})$$

$$= \{F(x) - F(x, y)\} \{F(y) - F(x, y)\} F(x, y) \{1 - F(x) - F(y) + F(x, y)\}.$$

It is easy to check that  $c(x, y) - 2d(x, y) = \{F_{XY}(x, y) - F_X(x)F_Y(y)\}^2$  and thus

$$D = \int_{\mathbb{R}^2} c(x, y) - 2d(x, y) \, dF_{XY}(x, y). \quad (\text{B.5})$$

Interestingly  $4\{c(x, y) - 2d(x, y)\} = \tau^*\{1_{(X \leq x)}, 1_{(Y \leq y)}\}$  so that  $D$  can be interpreted as a weighted integral of  $\tau^*$  applied to discretized versions of the  $Z^i$ . This is the perspective taken in Appendix 5.2. Now

$$\begin{aligned} c^+(x, y) &= E\{1_{(X^1, X^2 \preceq x)} 1_{(X^3, X^4 \not\preceq x)} 1_{(Y^1, Y^2 \preceq y)} 1_{(Y^3, Y^4 \not\preceq y)}\}, \\ c^-(x, y) &= E\{1_{(X^1, X^2 \preceq x)} 1_{(X^3, X^4 \not\preceq x)} 1_{(Y^3, Y^4 \preceq y)} 1_{(Y^1, Y^2 \not\preceq y)}\}, \\ d(x, y) &= E\{1_{(X^1, X^2 \preceq x)} 1_{(X^3, X^4 \not\preceq x)} 1_{(Y^1, Y^3 \preceq y)} 1_{(Y^2, Y^4 \not\preceq y)}\} \\ &= E\{1_{(X^1, X^2 \preceq x)} 1_{(X^3, X^4 \not\preceq x)} 1_{(Y^2, Y^4 \preceq y)} 1_{(Y^1, Y^3 \not\preceq y)}\}. \end{aligned}$$

This gives

$$\begin{aligned} \int_{\mathbb{R}^{r+s}} c^+(x, y) dF_{XY}(x, y) &= \int_{\mathbb{R}^2} E\{1_{(X^1, X^2 \preceq x)} 1_{(X^3, X^4 \not\preceq x)} 1_{(Y^1, Y^2 \preceq y)} 1_{(Y^3, Y^4 \not\preceq y)}\} dF_{XY}(x, y) \\ &= E\left\{\int_{\mathbb{R}^{r+s}} 1_{(X^1, X^2 \preceq x)} 1_{(X^3, X^4 \not\preceq x)} 1_{(Y^1, Y^2 \preceq y)} 1_{(Y^3, Y^4 \not\preceq y)} dF_{XY}(x, y)\right\} \\ &= E\{1_{(X^1, X^2 \preceq X^5)} 1_{(X^3, X^4 \not\preceq X^5)} 1_{(Y^1, Y^2 \preceq Y^5)} 1_{(Y^3, Y^4 \not\preceq Y^5)}\} \\ &= E\{I_D(X^{[5]})I_D(Y^{[5]})\}. \end{aligned}$$

Similarly one may also show that

$$\begin{aligned} \int_{\mathbb{R}^2} c^-(x, y) dF_{XY}(x, y) &= E\{I_D(X^{[5]})I_D(Y^{4,3,2,1,5})\}, \\ \int_{\mathbb{R}^2} d(x, y) dF_{XY}(x, y) &= E\{I_D(X^{[5]})I_D(Y^{1,3,2,4,5})\} \\ &= E\{I_D(X^{[5]})I_D(Y^{4,2,3,1,5})\}. \end{aligned}$$

From this and Equation (B.5) it is easy to see that

$$D(X, Y) = E\{I_D(X^{[5]}) \sum_{\sigma \in H_{\tau^*}} \text{sign}(\sigma) I_D(Y^{[5]})\}.$$

Our claim then follows by Lemma 5.11. Following essentially identical steps as for  $D(X, Y)$ , one may also show our desired result for  $R(X, Y)$ .  $\square$

Without loss of generality let  $\mu$  be as in Equation (5.1).

We first show that  $\mu$  is nonparametric. Letting  $h_{X,i} : \mathbb{R} \rightarrow \mathbb{R}$  and  $h_{Y,j} : \mathbb{R} \rightarrow \mathbb{R}$  strictly increasing functions for  $i \in [r]$ ,  $j \in [s]$  and letting  $h_X(x) = (h_{X,1}[x_1], \dots, h_{X,r}[x_r])$  and  $h_Y(y) = (h_{Y,1}[y_1], \dots, h_{Y,s}[y_s])$  we wish to show that  $\mu(X, Y) = \mu\{h_X(X), h_Y(Y)\}$ .

It is trivial to check that, as the  $h_{X,i}$  and  $h_{Y,i}$  are strictly increasing we have that  $\mathcal{R}(X^{[m]}) = \mathcal{R}\{h_X(X^{[r]})\}$  and  $\mathcal{R}(Y^{[m]}) = \mathcal{R}\{h_Y(Y^{[s]})\}$ . Given this, the claim follows immediately as rank indicator functions depend on their inputs only through the joint ranks of the inputs.

Next we show that  $\mu$  is I-consistent. Recall that, by definition,  $H \subset S_m$  has an equal number of even and odd permutations. It follows then that

$$\sum_{\sigma \in H} \text{sign}(\sigma) = 0.$$

When  $X \perp\!\!\!\perp Y$ , since the  $X^{[m]}$  and  $Y^{[m]}$  are independent and identically distributed respectively, we have

$$\begin{aligned} \mu(X, Y) &= E \left[ \left\{ \sum_{\sigma \in H} \text{sign}(\sigma) I_X(X^{\sigma^{[m]}}) \right\} \left\{ \sum_{\sigma \in H} \text{sign}(\sigma) I_Y(Y^{\sigma^{[m]}}) \right\} \right] \\ &= E \left\{ I_X(X^{[m]}) \right\} E \left\{ I_Y(Y^{[m]}) \right\} \left\{ \sum_{\sigma \in H} \text{sign}(\sigma) \right\} \left\{ \sum_{\sigma \in H} \text{sign}(\sigma) \right\} \\ &= E \left\{ I_X(X^{[m]}) \right\} E \left\{ I_Y(Y^{[m]}) \right\} \cdot 0 \cdot 0 \\ &= 0 \end{aligned}$$

which proves the claim.

Finally we show that symmetric rank covariances are closed under products. Without loss of generality assume that  $\mu = \mu_{I_X, I_Y, H}$  and  $\nu = \mu_{\tilde{I}_X, \tilde{I}_Y, \tilde{H}}$ . We have that

$$\begin{aligned} \mu(X, Y) &= E \left[ \left\{ \sum_{\sigma \in H} \text{sign}(\sigma) I_X(X^{\sigma^{[m]}}) \right\} \left\{ \sum_{\sigma \in H} \text{sign}(\sigma) I_Y(Y^{\sigma^{[m]}}) \right\} \right], \\ \nu(X, Y) &= E \left[ \left\{ \sum_{\sigma \in \tilde{H}} \text{sign}(\sigma) \tilde{I}_X(X^{\sigma^{[n]}}) \right\} \left\{ \sum_{\sigma \in \tilde{H}} \text{sign}(\sigma) \tilde{I}_Y(Y^{\sigma^{[n]}}) \right\} \right]. \end{aligned}$$

In the following we will implicitly let  $I_X(x^{[m+n]}) = I_X(x^{[m]})$ ,  $I_Y(y^{[m+n]}) = I_Y(y^{[m]})$ ,  $\tilde{I}_X(x^{[m+n]}) = \tilde{I}_X(x^{[n]})$ , and  $\tilde{I}_Y(y^{[m+n]}) = \tilde{I}_Y(y^{[n]})$  so that these indicator functions drop unused inputs. Now let  $\gamma \in S_{[m+n]}$  be the permutation that cyclically shifts all elements  $n$  units to the right, so that  $i \in [m+n]$  is taken to  $i+n \pmod{m+n}$  by  $\gamma$ . Then let  $g_\gamma : \mathbb{R}^{d \times (m+n)} \rightarrow \mathbb{R}^{d \times (m+n)}$  be the function which acts on its input with  $\gamma$ , that is we let  $g_\gamma(w^{[m+n]}) = w^{\gamma[m+n]}$  for all  $w^{[m+n]} \in \mathbb{R}^{d \times (m+n)}$ . Then define

$$\bar{H} = \gamma^{-1} \tilde{H} \gamma, \quad \bar{I}_X = \tilde{I}_X \circ g_\gamma, \quad \text{and} \quad \bar{I}_Y = \tilde{I}_Y \circ g_\gamma.$$

Clearly  $\bar{H}$  is a subgroup of  $S_{m+n}$  and it is easy to check that

$$\nu(X, Y) = E \left[ \left\{ \sum_{\sigma \in \bar{H}} \text{sign}(\sigma) \bar{I}_X(X^{\sigma[m+n]}) \right\} \left\{ \sum_{\sigma \in \bar{H}} \text{sign}(\sigma) \bar{I}_Y(Y^{\sigma[m+n]}) \right\} \right].$$

Now

$$\begin{aligned} A &= \left\{ \sum_{\sigma \in H} \text{sign}(\sigma) I_X(X^{\sigma[m+n]}) \right\} \left\{ \sum_{\sigma \in H} \text{sign}(\sigma) I_Y(Y^{\sigma[m+n]}) \right\}, \\ B &= \left\{ \sum_{\sigma \in \bar{H}} \text{sign}(\sigma) \bar{I}_X(X^{\sigma[m+n]}) \right\} \left\{ \sum_{\sigma \in \bar{H}} \text{sign}(\sigma) \bar{I}_Y(Y^{\sigma[m+n]}) \right\} \end{aligned}$$

depend only on  $Z^{[m+n]}$  through the entries  $Z^{[m]}$  and  $Z^{m+1, \dots, m+n}$  respectively, it thus follows that  $A$  and  $B$  are independent. Thus, by how we have defined  $\bar{I}_X, \bar{I}_Y$  and  $\bar{H}$ , we have that

$$\begin{aligned} \mu \nu &= E(A)E(B) \\ &= E(AB) \\ &= \left\{ \sum_{\substack{\sigma \in H \\ \bar{\sigma} \in \bar{H}}} \text{sign}(\sigma \bar{\sigma}) (I_X \bar{I}_X)(X^{(\sigma \bar{\sigma})[m+n]}) \right\} \left\{ \sum_{\substack{\sigma \in H \\ \bar{\sigma} \in \bar{H}}} \text{sign}(\sigma \bar{\sigma}) (I_Y \bar{I}_Y)(Y^{(\sigma \bar{\sigma})[m+n]}) \right\} \\ &= \left\{ \sum_{\sigma \in H \tilde{H}} \text{sign}(\sigma) (I_X \bar{I}_X)(X^{\sigma[m+n]}) \right\} \left\{ \sum_{\sigma \in H \tilde{H}} \text{sign}(\sigma) (I_Y \bar{I}_Y)(Y^{\sigma[m+n]}) \right\}, \end{aligned}$$

where the last line follows since that  $H \cap \bar{H} = \{e\}$  implies that  $|H\bar{H}| = |H||\bar{H}|$  and since elements of  $H$  and  $\bar{H}$  commute we have that  $H\bar{H}$  is a subgroup of  $S_{[m+n]}$ . The above equality shows that  $\mu\nu$  is a symmetric rank covariance as claimed.  $\square$

## PROOF OF LEMMA 5.11

For any  $\gamma \in H$ , by relabeling  $Z^{[m]}$  as  $Z^{\gamma^{-1}[m]}$ , we have that

$$\begin{aligned}
& E \left\{ \text{sign}(\gamma) I_X(X^{\gamma[m]}) \sum_{\sigma \in H} \text{sign}(\sigma) I_Y(Y^{\sigma[m]}) \right\} \\
&= E \left\{ I_X(X^{\gamma\gamma^{-1}[m]}) \sum_{\sigma \in H} \text{sign}(\sigma) \text{sign}(\gamma) I_Y(Y^{\sigma\gamma^{-1}[m]}) \right\} \\
&= E \left\{ I_X(X^{[m]}) \sum_{\sigma \in H} \text{sign}(\sigma\gamma^{-1}) I_Y(Y^{\sigma\gamma^{-1}[m]}) \right\} \\
&= E \left\{ I_X(X^{[m]}) \sum_{\sigma \in H} \text{sign}(\sigma) I_Y(Y^{\sigma[m]}) \right\}
\end{aligned}$$

where the third equality holds since  $\text{sign}(\gamma) = \text{sign}(\gamma^{-1})$  and the fourth equality holds since  $\gamma \in H \implies H = H\gamma^{-1}$ . Now plugging the above equality into our definition of  $\mu(X, Y)$  gives Equation (5.3). By symmetry we obtain Equation (5.4).  $\square$

## B.2.2 Proofs for Section 5.2

## PROOF OF PROPOSITION 5.14

Block minors of  $M(x, y)$  include the usual  $2 \times 2$  minors and thus if all such block minors vanish we have  $B^X(x) \perp\!\!\!\perp B^Y(y)$  by the discussion below Definition B5.12. Now suppose that  $B^X(x) \perp\!\!\!\perp B^Y(y)$  and let  $L, L' \subset \{0, 1\}^r$  and  $R, R' \subset \{0, 1\}^s$ . Then we have that

$$\begin{aligned}
& \left\{ \sum_{\substack{\ell_X \in L \\ \ell_Y \in R}} p(z)_{\ell_X \ell_Y} \right\} \left\{ \sum_{\substack{\ell'_X \in L' \\ \ell'_Y \in R'}} p(z)_{\ell'_X \ell'_Y} \right\} - \left\{ \sum_{\substack{\ell'_X \in L' \\ \ell'_Y \in R}} p(z)_{\ell'_X \ell'_Y} \right\} \left\{ \sum_{\substack{\ell_X \in L \\ \ell_Y \in R}} p(z)_{\ell_X \ell_Y} \right\} \\
&= P\{B^X(x) \in L, B^Y(y) \in R\} P\{B^X(x) \in L', B^Y(y) \in R'\} \\
&\quad - P\{B^X(x) \in L', B^Y(y) \in R\} P\{B^X(x) \in L, B^Y(y) \in R'\} \\
&= P\{B^X(x) \in L\} P\{B^Y(y) \in R\} P\{B^X(x) \in L'\} P\{B^Y(y) \in R'\} \\
&\quad - P\{B^X(x) \in L'\} P\{B^Y(y) \in R\} P\{B^X(x) \in L\} P\{B^Y(y) \in R'\} \\
&= 0
\end{aligned}$$

by independence.  $\square$

## PROOF OF PROPOSITION 5.16

Recall that for any  $d \geq 1$ ,  $0_d \in \mathbb{R}^d$  is the vector of all zeros. Let  $d = r + s$ . By definition and simple algebra

$$\begin{aligned} A(x, y)^2 &= \left[ \sum_{\substack{\ell_X \in L \\ \ell_Y \in R}} \{p(z)_{0_d} p(z)_{\ell_X \ell_Y} - p(z)_{\ell_X 0_s} p(z)_{0_r \ell_Y}\} \right]^2 \\ &= p(z)_{0_d}^2 \left\{ \sum_{\substack{\ell_X \in L \\ \ell_Y \in R}} p(z)_{\ell_X \ell_Y} \right\}^2 + \left\{ \sum_{\ell_X \in L} p(z)_{\ell_X 0_s} \right\}^2 \left\{ \sum_{\ell_Y \in R} p(z)_{0_r \ell_Y} \right\}^2 \\ &\quad - 2 p(z)_{0_d} \left\{ \sum_{\substack{\ell_X \in L \\ \ell_Y \in R}} p(z)_{\ell_X \ell_Y} \right\} \left\{ \sum_{\ell_X \in L} p(z)_{\ell_X 0_s} \right\} \left\{ \sum_{\ell_Y \in R} p(z)_{0_r \ell_Y} \right\}. \end{aligned}$$

Also, since  $\lambda_{XY}(x, y) = \prod_{i=1}^t F_{X_{E_i} Y_{F_i}}(x_{E_i}, y_{F_i})$ ,  $\lambda_{XY}$  is the cumulative distribution function of a random vector in  $\mathbb{R}^{r+s}$  whose entries are taken from  $Z^{5, \dots, 4+t}$ , in particular we may, for  $j \in [r + s]$ , let

$$W_j = \begin{cases} X^{4+k} & j \in [r] \text{ and } j \in E_k, \quad \text{and} \\ Y^{4+k} & r + 1 \leq j \leq r + s \text{ and } j - r \in F_k. \end{cases}$$

Here  $W$  is just a projection of  $Z^{5, \dots, 4+t}$ . Given this fact we have that, for any integrable function  $g$ ,  $\int_{\mathbb{R}^{r+s}} g(z) d\lambda_{XY} = E[g(W)]$ . Now, by a direct computation, we have that

$$\begin{aligned} &\int_{\mathbb{R}^{r+s}} p(z)_{0_d}^2 \left\{ \sum_{\substack{\ell_X \in L \\ \ell_Y \in R}} p(z)_{\ell_X \ell_Y} \right\}^2 d\lambda_{XY}(x, y) \\ &= \int_{\mathbb{R}^{r+s}} E \left[ \mathbf{1}_{(Z^1, Z^2 \preceq z)} \left\{ \sum_{\ell_X \in L} \mathbf{1}_{(X^3 \preceq_{\ell_X} x)} \right\} \left\{ \sum_{\ell_X \in L} \mathbf{1}_{(X^4 \preceq_{\ell_X} x)} \right\} \right. \\ &\quad \left. \left\{ \sum_{\ell_Y \in R} \mathbf{1}_{(Y^3 \preceq_{\ell_Y} y)} \right\} \left\{ \sum_{\ell_Y \in R} \mathbf{1}_{(Y^4 \preceq_{\ell_Y} y)} \right\} \right] d\lambda_{XY}(x, y) \\ &= E \left[ \mathbf{1}_{(Z^1, Z^2 \preceq W)} \left\{ \sum_{\ell_X \in L} \mathbf{1}_{(X^3 \preceq_{\ell_X} W^X)} \right\} \left\{ \sum_{\ell_X \in L} \mathbf{1}_{(X^4 \preceq_{\ell_X} W^X)} \right\} \right. \\ &\quad \left. \left\{ \sum_{\ell_Y \in R} \mathbf{1}_{(Y^3 \preceq_{\ell_Y} W^Y)} \right\} \left\{ \sum_{\ell_Y \in R} \mathbf{1}_{(Y^4 \preceq_{\ell_Y} W^Y)} \right\} \right] \\ &= E \left\{ I_X(X^{[4+t]}) I_Y(Y^{[4+t]}) \right\}. \end{aligned}$$

Similarly we have that

$$\int_{\mathbb{R}^{r+s}} \left\{ \sum_{\ell_X \in L} p(z)_{\ell_X 0_s} \right\}^2 \left\{ \sum_{\ell_Y \in R} p(z)_{0_r \ell_Y} \right\}^2 d\lambda_{XY}(x, y) = E \left\{ I_X(X^{[4+t]}) I_Y(Y^{4,2,3,1,5,\dots,t}) \right\}$$

and

$$\begin{aligned} & \int_{\mathbb{R}^{r+s}} p(z)_{0_d} \left\{ \sum_{\substack{\ell_X \in L \\ \ell_Y \in R}} p(z)_{\ell_X \ell_Y} \right\} \left\{ \sum_{\ell_X \in L} p(z)_{\ell_X 0_s} \right\} \left\{ \sum_{\ell_Y \in R} p(z)_{0_r \ell_Y} \right\} d\lambda_{XY}(x, y) \\ &= E \left\{ I_X(X^{[4+t]}) I_Y(Y^{1,3,2,4,5,\dots,t}) \right\} \\ &= E \left\{ I_X(X^{[4+t]}) I_Y(Y^{4,2,3,1,5,\dots,t}) \right\}. \end{aligned}$$

Thus

$$\begin{aligned} & \int_{\mathbb{R}^{r+s}} A(x, y)^2 d\lambda_{XY}(x, y) \\ &= E \left[ I_X(X^{[4+t]}) \left\{ I_Y(Y^{[4+t]}) + I_Y(Y^{4,2,3,1,5,\dots,t}) - I_Y(Y^{4,2,3,1,5,\dots,t}) - I_Y(Y^{1,3,2,4,5,\dots,t}) \right\} \right]. \end{aligned}$$

Our result then follows by Lemma 5.11.

It now remains to show that  $D$  and  $R$  are integrated squared minors. But this is easy, recall from the proof of Proposition 5.6 that, omitting subscripts for space,

$$\begin{aligned} & \{F(x, y) - F(x)F(y)\}^2 \\ &= F(x, y)^2 \{1 - F(x) - F(y) + F(x, y)\}^2 + \{F(x) - F(x, y)\}^2 \{F(y) - F(x, y)\}^2 \\ &\quad - 2 F(x, y) \{1 - F(x) - F(y) + F(x, y)\} \{F(x) - F(x, y)\} \{F(y) - F(x, y)\} \\ &= c^+(x, y) + c^-(x, y) - 2d(x, y) \end{aligned}$$

where  $c^+$ ,  $c^-$ , and  $d$  are given by Equations (B.1)–(B.4). But

$$\begin{aligned} F_{XY}(x, y) &= p(z)_{0_d}, \\ F_Y(y) - F_{XY}(x, y) &= \sum_{\ell_X \in \{0,1\}^r \setminus \{0_r\}} p(z)_{\ell_X 0_s}, \\ F_X(x) - F_{XY}(x, y) &= \sum_{\ell_Y \in \{0,1\}^s \setminus \{0_s\}} p(z)_{0_r \ell_Y}, \\ 1 - F_X(x) - F_Y(y) + F_{XY}(x, y) &= \sum_{\substack{\ell_X \in \{0,1\}^r \setminus \{0_r\} \\ \ell_Y \in \{0,1\}^s \setminus \{0_s\}}} p(z)_{\ell_X \ell_Y}. \end{aligned}$$

Thus  $\{F_{XY}(x, y) - F_X(x)F_Y(y)\}^2$  equals the square of the  $2 \times 2$  block minor of  $M(x, y)$  along  $(\{0_r\}, \{0, 1\}^r \setminus \{0_r\}, \{0_s\}, \{0, 1\}^s \setminus \{0_s\})$ . That is, we have

$$\begin{aligned} D(X, Y) &= \int_{\mathbb{R}^{r+s}} \left[ \sum_{\substack{\ell_X \in \{0, 1\}^r \setminus \{0\} \\ \ell_Y \in \{0, 1\}^s \setminus \{0\}}} \{p(z)_{0_d} p(z)_{\ell_X \ell_Y} - p(z)_{0_r \ell_Y} p(z)_{\ell_X 0_s}\} \right]^2 dF_{XY}(x, y) \quad (\text{B.6}) \\ &= \int_{\mathbb{R}^{r+s}} A(x, y)^2 dF_{XY}(x, y). \end{aligned}$$

Thus  $D(X, Y)$  is indeed an integrated squared minor as claimed. That  $R(X, Y)$  is an integrated squared minor follows in exactly the same way.  $\square$

### PROOF OF PROPOSITION 5.17

All  $\mu_i^{joint}, \mu_i^{prod}$  are symmetric rank covariances by Proposition B5.16. It then follows, by definition, that  $\mu^{joint}$  and  $\mu^{prod}$  are summed symmetric rank covariances. We first show that  $\mu^{joint} = 0 \implies D = 0$  so that  $\mu^{joint}$  is consistent whenever  $D$  is. Recalling (B.6) and the fact that the  $L_i \times R_i$  partition  $(\{0, 1\}^r \setminus \{0_r\}) \times (\{0, 1\}^s \setminus \{0_s\})$  we have that

$$\begin{aligned} D(X, Y) &= \int_{\mathbb{R}^{r+s}} \left[ \sum_{\substack{\ell_X \in \{0, 1\}^r \setminus \{0_r\} \\ \ell_Y \in \{0, 1\}^s \setminus \{0_s\}}} \{p(z)_{0_d} p(z)_{\ell_X \ell_Y} - p(z)_{0_r \ell_Y} p(z)_{\ell_X 0_s}\} \right]^2 dF_{XY}(x, y) \\ &= \int_{\mathbb{R}^{r+s}} \left[ \sum_{i=1}^k \sum_{\substack{\ell_X \in L_i \\ \ell_Y \in R_i}} \{p(z)_{0_d} p(z)_{\ell_X \ell_Y} - p(z)_{0_r \ell_Y} p(z)_{\ell_X 0_s}\} \right]^2 dF_{XY}(x, y). \end{aligned}$$

Now recall that if  $a, b \in \mathbb{R}$  then  $(a + b)^2 > 0 \implies a^2 + b^2 > 0$ . Applying this fact  $k$  times we have that

$$\begin{aligned} &\left[ \sum_{i=1}^k \sum_{\substack{\ell_X \in L_i \\ \ell_Y \in R_i}} \{p(z)_{0_d} p(z)_{\ell_X \ell_Y} - p(z)_{0_r \ell_Y} p(z)_{\ell_X 0_s}\} \right]^2 > 0 \\ \implies &\sum_{i=1}^k \left[ \sum_{\substack{\ell_X \in L_i \\ \ell_Y \in R_i}} \{p(z)_{0_d} p(z)_{\ell_X \ell_Y} - p(z)_{0_r \ell_Y} p(z)_{\ell_X 0_s}\} \right]^2 > 0. \end{aligned}$$

From this it immediately follows that  $\mu^{joint} = 0 \implies D = 0$  as claimed. An essentially identical argument shows that  $\mu^{prod} = 0 \implies R = 0$ . Since  $R$  is D-consistent in all cases this implies that  $\mu^{prod}$  is also.  $\square$

### B.3 Proofs for Chapter 6

#### PROOF OF PROPOSITION 6.1

We will only show Equation (6.3), Equation (6.4) then follows by symmetry. Now

$$\begin{aligned}
\kappa(z^{[m]}) &= \frac{1}{m!} \sum_{\gamma \in S_m} \left\{ \sum_{\sigma \in H} \text{sign}(\sigma) I_X(x^{\sigma\gamma^{[m]}}) \right\} \left\{ \sum_{\sigma \in H} \text{sign}(\sigma) I_Y(y^{\sigma\gamma^{[m]}}) \right\} \\
&= \frac{1}{m!} \sum_{\sigma \in H} \sum_{\gamma \in S_m} \text{sign}(\sigma) I_X(x^{\sigma\gamma^{[m]}}) \left\{ \sum_{\psi \in H} \text{sign}(\psi) I_Y(y^{\psi\gamma^{[m]}}) \right\} \\
&= \frac{1}{m!} \sum_{\sigma \in H} \sum_{\sigma^{-1}\gamma \in S_m} \text{sign}(\sigma) I_X(x^{\sigma\sigma^{-1}\gamma^{[m]}}) \left\{ \sum_{\psi \in H} \text{sign}(\psi) I_Y(y^{\psi\sigma^{-1}\gamma^{[m]}}) \right\} \\
&= \frac{1}{m!} \sum_{\sigma \in H} \sum_{\sigma^{-1}\gamma \in S_m} I_X(x^{\gamma^{[m]}}) \left\{ \sum_{\psi \in H} \text{sign}(\psi)\text{sign}(\sigma) I_Y(y^{\psi\sigma^{-1}\gamma^{[m]}}) \right\} \\
&= \frac{1}{m!} \sum_{\sigma \in H} \sum_{\sigma^{-1}\gamma \in S_m} I_X(x^{\gamma^{[m]}}) \left\{ \sum_{\psi \in H} \text{sign}(\psi\sigma^{-1}) I_Y(y^{(\psi\sigma^{-1})\gamma^{[m]}}) \right\} \\
&= \frac{1}{m!} \sum_{\sigma \in H} \sum_{\sigma^{-1}\gamma \in S_m} I_X(x^{\gamma^{[m]}}) \left\{ \sum_{\psi \in H} \text{sign}(\psi) I_Y(y^{\psi\gamma^{[m]}}) \right\} \\
&= \frac{|H|}{m!} \sum_{\gamma \in S_m} I_X(x^{\gamma^{[m]}}) \left\{ \sum_{\psi \in H} \text{sign}(\psi) I_Y(y^{\psi\gamma^{[m]}}) \right\},
\end{aligned}$$

where we have used the fact that for any  $\sigma, \psi \in H$ ,  $\sigma H = H$  and  $\sigma S_m = S_m$ ,  $\text{sign}(\psi\sigma^{-1}) = \text{sign}(\psi)\text{sign}(\sigma^{-1})$ , and  $\text{sign}(\sigma) = \text{sign}(\sigma^{-1})$ .  $\square$

### B.4 Proofs for Chapter 7

#### PROOF OF LEMMA 7.3

Without loss of generality assume that  $S = \{\ell+1, \dots, m\}$ . Moreover let  $W^i = (W_X^i, W_Y^i)$  be a partition of  $W^i$  into its  $X$  and  $Y$  components. We wish to show that  $E\{k(Z^{[\ell]}, z^{\ell+1, \dots, m})\} = 0$ .

By  $X \perp\!\!\!\perp Y$  we have that

$$E\{k(W)\} = E\left\{ \sum_{\sigma \in H} \text{sign}(\sigma) I_X(W_X^{\sigma^{[m]}}) \right\} E\left\{ \sum_{\sigma \in H} \text{sign}(\sigma) I_Y(W_Y^{\sigma^{[m]}}) \right\}.$$

Now, letting  $\tau_i \in E_i$  be a representative of the  $i$ th equivalence class, we have

$$\begin{aligned}
E\left\{\sum_{\sigma \in H} \text{sign}(\sigma) I_X(W_X^{\sigma[m]})\right\} &= E\left\{\sum_{i=1}^t \sum_{\sigma \in E_i} \text{sign}(\sigma) I_X(W_X^{\sigma[m]})\right\} \\
&= \sum_{i=1}^t \sum_{\sigma \in E_i} \text{sign}(\sigma) E\{I_X(W_X^{\sigma[m]})\} \\
&= \sum_{i=1}^t E\{I_X(W_X^{\tau_i[m]})\} \sum_{\sigma \in E_i} \text{sign}(\sigma) \\
&= \sum_{i=1}^t E\{I_X(W_X^{\tau_i[m]})\} 0 \\
&= 0
\end{aligned}$$

where the third equality follows since the  $X^i$  are independent and identically distributed and so we may relabel them in  $W_X^{\sigma[m]}$  so long as we preserve the locations of the  $x_i$  and the fourth equality follows as each  $E_i$  contains an equal number of even and odd permutations. It follows that  $E[k(W)] = 0$ .  $\square$

#### PROOF OF PROPOSITION 7.4

By Lemma 7.3,  $E[k\{\sigma(z^1, Z^2, \dots, Z^m)\}] = 0$  for all  $\sigma \in S_m$ . Hence,

$$\kappa_1(z^1) = E\{\kappa(z^1, Z^2, Z^3, \dots, Z^m)\} = \frac{1}{m!} \sum_{\sigma \in S_m} E[k\{\sigma(z^1, Z^2, \dots, Z^m)\}] = 0.$$

$\square$

#### PROOF OF LEMMA 7.5

We first show that  $\kappa_1(z^1) \equiv 0$  so that  $U_\mu$  is degenerate. To see this let  $S = \{i\}$  for some  $i \in [m]$ . If  $i > 4$  then every element of  $h \in H_{\tau^*}$  fixes  $i$  and hence, using Lemma 7.3 with  $g = e$ , we see that all  $h \in H_{\tau^*}$  are in the same equivalence class. It follows that said equivalence class has an equal number of even and odd permutations and thus  $E\{k(Z^1, \dots, z^{i-1}, z^i, Z^{i+1}, \dots, Z^m)\} = 0$ . Now suppose that  $i \leq 4$ . Using Lemma 7.3 it is easy to check, using the fact that the

invariance group of  $\mu$  contains  $G$ , that  $H_{\tau^*}$  is divided into two equivalence classes both of which contain an even and an odd permutation and thus Lemma 7.3 holds. Since Lemma 7.3 holds whenever  $S$  is a singleton set, it follows, by Proposition 7.4, that  $U_\mu$  is degenerate as claimed.

We now show that  $\kappa_2$  has the claimed form. Recall that

$$\kappa_2(z^1, z^2) = E\{\kappa(z^1, z^2, Z^3, \dots, z^m)\} \quad (\text{B.7})$$

$$= \frac{1}{m!} \sum_{\sigma \in S_m} E[k\{\sigma(z^1, z^2, Z^3, \dots, z^m)\}]. \quad (\text{B.8})$$

Suppose that  $\sigma \in S_m$  is such that  $S = \{\sigma(1), \sigma(2)\} \not\subset [4]$ . Then we must have that either  $\sigma(1)$  or  $\sigma(2)$  is fixed by all elements in  $h \in H_{\tau^*}$ . It is then easy to check that, similarly as above, the conditions of Lemma 7.3 hold for  $S$  and thus  $E[k\{\gamma(z^1, z^2, Z^3, \dots, z^m)\}] = 0$ . Hence we have that

$$\kappa_2(z^1, z^2) = \frac{1}{m!} \sum_{\substack{\sigma \in S_m \\ \sigma(1), \sigma(2) \in [4]}} E[k\{\sigma(z^1, z^2, Z^3, \dots, z^m)\}].$$

As the  $Z^i$  are independent and identically distributed and thus exchangeable it follows that, for any  $\sigma, \gamma \in S_m$ , if  $\sigma(i) = \gamma(i)$  for  $i = 1, 2$  then

$$E[k\{\sigma(z^1, z^2, Z^3, \dots, z^m)\}] = E[k\{\gamma(z^1, z^2, Z^3, \dots, z^m)\}].$$

This allows us to write

$$\kappa_2(z^1, z^2) = \frac{(m-2)!}{m!} \sum_{\substack{\sigma \in S_4 \\ \sigma(3) < \sigma(4)}} E\{k(\sigma(z^1, z^2, Z^3, Z^4), Z^5, \dots, z^m)\}.$$

Now

$$\begin{aligned} & \sum_{\substack{\sigma \in S_4 \\ \sigma(3) < \sigma(4) \\ \sigma(1) < \sigma(2)}} E\{k(\sigma(z^1, z^2, Z^3, Z^4), Z^5, \dots, z^m)\} \\ &= E\{k(z^1, z^2, Z^3, Z^4, Z^5, \dots, z^m)\} + E\{k(z^1, Z^3, z^2, Z^4, Z^5, \dots, z^m)\} \\ &+ E\{k(z^1, Z^3, Z^4, z^2, Z^5, \dots, z^m)\} + E\{k(Z^3, z^1, z^2, Z^4, Z^5, \dots, z^m)\} \\ &+ E\{k(Z^3, z^1, Z^4, z^2, Z^5, \dots, z^m)\} + E\{k(Z^3, Z^4, z^1, z^2, Z^5, \dots, z^m)\}. \end{aligned}$$

By definition of  $k$  it is easy to verify, using the fact that  $G$  is a subset of the invariance group, that

$$E\{k(z^1, Z^3, Z^4, z^2, Z^5, \dots, m)\} = E\{k(Z^3, z^1, z^2, Z^4, Z^5, \dots, m)\} = 0$$

and

$$\begin{aligned} E\{k(z^1, z^2, Z^3, Z^4, Z^5, \dots, m)\} &= E\{k(z^1, Z^3, z^2, Z^4, Z^5, \dots, m)\} \\ &= E\{k(Z^3, z^1, Z^4, z^2, Z^5, \dots, m)\} = E\{k(Z^3, Z^4, z^1, z^2, Z^5, \dots, m)\}. \end{aligned}$$

Thus

$$\sum_{\substack{\sigma \in S_4 \\ \sigma(3) < \sigma(4) \\ \sigma(1) < \sigma(2)}} E\{k(\sigma(z^1, z^2, Z^3, Z^4), Z^5, \dots, m)\} = 4E\{k(z^1, z^2, Z^3, Z^4, Z^5, \dots, m)\}.$$

By symmetry and as one may easily check that

$$E\{k(z^1, z^2, Z^3, Z^4, Z^5, \dots, m)\} = E\{k(z^2, z^1, Z^3, Z^4, Z^5, \dots, m)\}$$

we have

$$\begin{aligned} \kappa_2(z^1, z^2) &= \frac{(m-2)!}{m!} \sum_{\substack{\sigma \in S_4 \\ \sigma(3) < \sigma(4)}} E\{k(\sigma(z^1, z^2, Z^3, Z^4), Z^5, \dots, m)\} \\ &= \frac{(m-2)!}{m!} \left[ \sum_{\substack{\sigma \in S_4 \\ \sigma(3) < \sigma(4) \\ \sigma(1) < \sigma(2)}} E\{k(\sigma(z^1, z^2, Z^3, Z^4), Z^5, \dots, m)\} \right. \\ &\quad \left. + \sum_{\substack{\sigma \in S_4 \\ \sigma(3) < \sigma(4) \\ \sigma(2) < \sigma(1)}} E\{k(\sigma(z^1, z^2, Z^3, Z^4), Z^5, \dots, m)\} \right] \\ &= \frac{(m-2)!}{m!} \left[ 4E\{k(z^1, z^2, Z^3, Z^4, Z^5, \dots, m)\} + 4E\{k(z^2, z^1, Z^3, Z^4, Z^5, \dots, m)\} \right] \\ &= \frac{8(m-2)!}{m!} E\{k(z^1, z^2, Z^3, Z^4, Z^5, \dots, m)\} \\ &= \frac{4}{\binom{m}{2}} E\{k(z^1, z^2, Z^3, Z^4, Z^5, \dots, m)\}. \end{aligned}$$

□

## PROOF OF LEMMA 7.6

Let  $\varphi_{i,1}, \varphi_{i,2}, \dots$  be the sequence of orthonormal eigenfunctions associated with the nonzero eigenvalues  $\lambda_{i,1}, \lambda_{i,2}, \dots$  of  $A_{g_i}$ , for  $i = 1, 2$ . Since  $X \perp Y$ , for each  $(j_1, j_2) \in \mathbb{N}_+^2$ ,

$$\begin{aligned} & E[k((x_1, y_1), (X_2, Y_2))\varphi_{1,j_1}(X_2)\varphi_{2,j_2}(Y_2)] \\ &= E[g_1(x_1, X_2)g_2(y_1, Y_2)\varphi_{1,j_1}(X_2)\varphi_{2,j_2}(Y_2)] \\ &= E[g_1(x_1, X_2)\varphi_{1,j_1}(X_2)] E[g_2(y_1, Y_2)\varphi_{2,j_2}(Y_2)] \\ &= \lambda_{1,j_1}\varphi_{1,j_1}(x_1)\lambda_{2,j_2}\varphi_{2,j_2}(y_1). \end{aligned}$$

Therefore, for each  $(j_1, j_2) \in \mathbb{N}_+^2$ ,  $\lambda_{1,j_1}\lambda_{2,j_2}$  is an eigenvalue of  $A_k$  with the associated eigenfunction  $\varphi_{1,j_1}\varphi_{2,j_2}$ . Further,  $\{\varphi_{1,j_1}\varphi_{2,j_2} : (j_1, j_2) \in \mathbb{N}_+^2\}$  is an orthonormal system, since both  $\{\varphi_{1,1}, \varphi_{1,2}, \dots\}$  and  $\{\varphi_{2,1}, \varphi_{2,2}, \dots\}$  are orthonormal systems, and  $X \perp Y$ .

Now suppose  $\{\gamma_1, \gamma_2, \dots\}$  is a sequence of all nonzero eigenvalues of  $A_k$  with the associated orthonormal sequence of eigenfunctions  $\{\psi_1, \psi_2, \dots\}$ . Then

$$\sum_{j=1}^n \gamma_j \psi_j((X_1, Y_1), (X_2, Y_2)) \xrightarrow{L^2} k((X_1, Y_1), (X_2, Y_2)).$$

By independence,

$$\begin{aligned} \sum_{j_1=1}^{\infty} \sum_{j_2=1}^{\infty} \lambda_{1,j_1}^2 \lambda_{2,j_2}^2 &= E[g_1(X_1, X_2)^2] E[g_2(Y_1, Y_2)^2] \\ &= E[(g_1(X_1, X_2)g_2(Y_1, Y_2))^2] \\ &= E[k((X_1, Y_1), (X_2, Y_2))^2] \\ &= \sum_{j=1}^{\infty} \gamma_j^2. \end{aligned}$$

Therefore, we conclude that, as a multi-set,  $\{\lambda_{1,j_1}\lambda_{2,j_2} : (j_1, j_2) \in \mathbb{N}_+^2\}$  contains all nonzero eigenvalues of  $A_k$  with the correct multiplicity.  $\square$   $\square$

## PROOF OF LEMMA 7.7

Any collection of i.i.d. continuous random variables has their rank vector following a uniform distribution. Since the function  $a_{I_r^*}$  depends on its arguments only through their ranks, we have that, for  $x_1, x_2 \in (0, 1)$ ,

$$g(x_1, x_2) := E\{a_{I_r^*}(x_1, x_2, X_3, X_4)\} = E\{a_{I_r^*}(x_1, x_2, Y_3, Y_4)\}.$$

Now recall from Equation (7.4)

$$\kappa_2^{\tau^*}(z^{[2]}) = \frac{2}{3}g(x_1, x_2)g(y_1, y_2)$$

and thus the proof is complete once the following claim is established:

$$g(x_1, x_2) = 3c(x_1, x_2), \quad (x_1, x_2 \in (0, 1)). \quad (\text{B.9})$$

Letting  $x_{(1)} = x_1 \wedge x_2 = \min\{x_1, x_2\}$  and  $x_{(2)} = x_1 \vee x_2 = \max\{x_1, x_2\}$ , we have

$$\begin{aligned} g(x_1, x_2) &= P(x_1, x_2 < X_3, X_4) + P(x_1, x_2 > X_3, X_4) \\ &\quad - P(x_1, X_3 < x_2, X_4) - P(x_1, X_3 > x_2, X_4) \\ &= P(x_{(2)} < X_3, X_4) + P(x_{(1)} > X_3, X_4) - P(x_{(1)}, X_3 < x_{(2)}, X_4) \\ &= (1 - x_{(2)})^2 + x_{(1)}^2 - P(x_{(1)}, X_3 < x_{(2)}, X_4). \end{aligned}$$

Moreover,

$$\begin{aligned} P(x_{(1)}, X_3 < x_{(2)}, X_4) &= P(x_{(1)} < X_4 \text{ and } X_3 < x_{(1)}) \\ &\quad + P(X_3 < X_4 \text{ and } x_{(1)} < X_3 < x_{(2)}) \\ &= x_{(1)}(1 - x_{(1)}) + \int_{x_{(1)}}^{x_{(2)}} P(x < X_4 \mid X_3 = x) \, dx \\ &= x_{(1)}(1 - x_{(1)}) + \int_{x_{(1)}}^{x_{(2)}} (1 - x) \, dx \\ &= x_{(1)}(1 - x_{(1)}) + x_{(2)} \left(1 - \frac{1}{2}x_{(2)}\right) - x_{(1)} \left(1 - \frac{1}{2}x_{(1)}\right). \end{aligned}$$

We obtain that

$$g(x_1, x_2) = 1 + \frac{3}{2}x_{(1)}^2 + \frac{3}{2}x_{(2)}^2 - 3x_{(2)} = 1 + \frac{3}{2}x_1^2 + \frac{3}{2}x_2^2 - 3x_{(2)},$$

which is the claim from (B.9). □

PROOF OF THEOREM 7.8

Let  $c$  be the kernel function for the Cramér-von Mises statistic, as defined in Lemma 7.7. The operator  $A_c$  is known to have eigenvalues  $\frac{1}{j^2\pi^2}$  with corresponding eigenfunctions  $\sqrt{2}\cos(\pi jx)$  for  $j = 1, 2, \dots$  (van der Vaart, 1998, Example 12.13). Since  $\kappa_2^{\tau^*}(z^{[2]}) = 6c(x_1, x_2)c(y_1, y_2)$  by Lemma 7.7, it follows from Lemma 7.6 that  $\frac{1}{6}\kappa_2^{\tau^*}$  has eigenvalues  $\{\frac{1}{\pi^4 j^2 i^2} : (i, j) \in \mathbb{N}_+^2\}$  corresponding to orthonormal eigenfunctions  $\{2\cos(\pi jx)\cos(\pi jy) : (i, j) \in \mathbb{N}_+^2\}$ . The eigenvalues of  $\kappa_2^{\tau^*}$  are a multiple of 6 larger, with the same orthonormal eigenfunctions. We obtain from Theorem 7.2 that

$$nU_{\tau^*} \xrightarrow{d} \binom{4}{2} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{1}{\pi^4 j^2 i^2} (\chi_{1,ij}^2 - 1) = \frac{36}{\pi^4} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{1}{j^2 i^2} (\chi_{1,ij}^2 - 1)$$

where  $\{\chi_{1,ij}^2 : i, j \in \mathbb{N}_+\}$  is a collection of i.i.d.  $\chi_1^2$  random variables. □ □

PROOF OF PROPOSITION 7.9

Let  $\kappa^D, \kappa^R$  be the symmetrized kernels corresponding to  $D$  and  $R$  respectively. We will now show that  $\kappa_2^D$  and  $\kappa_2^R$  are scalar multiples of  $\kappa_2^{\tau^*}$ . By Lemma 7.5 we have that

$$\kappa_2^{\tau^*}(z^1, z^2) = \frac{2}{3} E\{a_{I_{\tau^*}}(x^1, x^2, X^3, X^4)\} E\{a_{I_{\tau^*}}(y^1, y^2, Y^3, Y^4)\}.$$

By Lemma 7.5 and Proposition 5.6 we have that

$$\kappa_2^D(z^1, z^2) = \frac{1}{10} E\{a_{I_D}(x^{1,2}, X^{3,4,5})\} E\{a_{I_D}(y^{1,2}, Y^{3,4,5})\}.$$

Now a lengthy but straightforward computation shows that

$$E\{a_{I_D}(x^{1,2}, X^{3,4,5})\} = \frac{1}{3} E\{a_{I_{\tau^*}}(x^{1,2}, X^{3,4})\}$$

and similarly for  $E\{a_{I_D}(y^{1,2}, Y^{3,4,5})\}$ . Thus

$$\kappa_2^D(z^1, z^2) = \frac{1}{90} E\{a_{I_{\tau^*}}(x^{1,2}, X^{3,4})\} E\{a_{I_{\tau^*}}(y^{1,2}, Y^{3,4})\} = \frac{1}{60} \kappa_2^{\tau^*}(z^1, z^2).$$

An essentially identical computation shows  $\kappa_2^R(z^1, z^2) = (1/90)\kappa_2^{\tau^*}(z^1, z^2)$ . Now, given knowledge of the eigenvalues of  $\kappa_2^{\tau^*}$  above, our results follow immediately from Theorem 7.2. □

PROOF OF THEOREM 7.10

Recall from Equation 7.4 that we have the factorization

$$\kappa_2^{\tau^*}(z^{[2]}) = \frac{2}{3} g_X(x_1, x_2) g_Y(y_1, y_2).$$

where

$$\begin{aligned} g_X(x_1, x_2) &:= E\{a_{I_{\tau^*}}(x^1, x^2, X^3, X^4)\}, \\ g_Y(y_1, y_2) &:= E\{a_{I_{\tau^*}}(y^1, y^2, Y^3, Y^4)\}. \end{aligned}$$

As in the proof of Theorem 7.8, finding the eigenvalues of  $\kappa_2^{\tau^*}$  requires only finding the eigenvalues of the operators  $A_{g_X}$  and  $A_{g_Y}$ . Obtaining the eigenvalues of  $A_{g_X}$  and  $A_{g_Y}$  are two analogous problems and we thus discuss only  $A_{g_X}$ . We denote the support of  $X$  by  $\{u_1, \dots, u_a\}$ .

Let  $F$  and  $p$  be the cumulative density function and probability mass function corresponding to  $X$  respectively. Using the fact that  $X_3$  and  $X_4$  are i.i.d. copies of  $X$ , we have that

$$\begin{aligned} k_X(x_1, x_2) &= P(x_1 \wedge x_2 > X)^2 + P(x_1 \vee x_2 < X)^2 - P(x_1 \wedge x_2, X_3 < x_1 \vee x_2, X_4) \\ &= \left[ (F(x_1 \wedge x_2) - p(x_1 \wedge x_2))^2 + (1 - F(x_1 \vee x_2))^2 \right] \\ &\quad - I(x_1 \neq x_2) \left[ F(x_1 \wedge x_2)(1 - F(x_1 \wedge x_2)) + \sum_{x_1 \wedge x_2 < u_\ell < x_1 \vee x_2} p(u_\ell)(1 - F(u_\ell)) \right]. \end{aligned}$$

Finding the eigenvalues of  $A_{g_X}$  requires finding  $\lambda \in \mathbb{R}$  and a function  $\varphi$  such that

$$\lambda \varphi(x) = E\{g_X(x, X_2)\varphi(X_2)\} = \sum_{j=1}^a p(u_j)\varphi(u_j)g_X(x, u_j), \quad (\text{B.10})$$

for  $x$  in the support of  $X$ . Since the support is finite, (B.10) is a system of  $a$  linear equations in  $a$  unknowns  $\varphi(u_1), \dots, \varphi(u_a)$ . We recognize that the eigenvalues of  $A_{g_X}$  are the eigenvalues of the  $a \times a$  matrix  $\tilde{R}^X$  whose  $(i, j)$ -th entry is  $g_X(u_i, u_j)p(u_j)$ .

Let  $K^X$  be the symmetric  $a \times a$  matrix with  $(i, j)$ -th entry  $g_X(u_i, u_j)$ , and let  $\text{diag}(p)$  be the diagonal  $a \times a$  matrix whose diagonal entries are  $p(u_1), \dots, p(u_a)$ . Then  $\tilde{R}^X = K^X \text{diag}(p)$ .

Noting that  $\tilde{R}^X$  has same eigenvalues as the symmetric matrix  $R^X = \text{diag}(p)^{1/2} K^X \text{diag}(p)^{1/2}$ , we obtain that the eigenvalues of  $A_{g_X}$  are the eigenvalues of  $R^X$ , which is the matrix given by (7.6). Since the analogous fact holds for  $g_Y$ , an application of Lemma 7.6 and Theorem 7.2 completes the proof.  $\square$

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