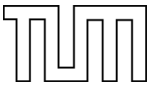

Technische Universität München

Department of Mathematics

Master's Thesis

Higher-order statistics for high-dimensional problems with applications to graphical models

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I hereby declare that this thesis is my own work and that no other sources have been used except those clearly indicated and referenced. This thesis was not previously presented to another examination board and has not been published.

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Abstract

A Gaussian graphical model is a statistical model, where the data follows a multivariate Normal distribution in which conditional independence relations of the random vector are encoded in a graph. Testing the hypothesis that a Gaussian graphical model is associated to either a graph or a specific subgraph corresponds to a composite hypothesis test in the Normal model. However, the standard likelihood ratio test for this problem has both poor power and size, and is only suitable if the sample size is large compared to the number of observations. In this thesis, we review higher-order approximations methods and apply them to subgraph testing in Gaussian graphical models. This allows us to define a transformation of the likelihood ratio statistic for which an accurate finite-sample distributional approximation is available. A simulation study shows that in settings of small and large sample sizes, the introduced statistical test is robust and favorable to the likelihood ratio test in terms of both power and size.

Contents

1 Introduction

With the democratization of data collection and analysis, the field of statistics is faced with new challenges stemming from the increased quantity and complexity of collected data. Graphical models have emerged in many scientific fields as a tool to describe variables of interest and their interactions. In biology, graphical models are used to study gene regulatory networks in order to better understand the development of diseases. In statistical mechanics, the Ising model [19] was introduced as a simplistic model of ferromagnetism to study interactions of particles on a 2-dimensional grid.

A *graphical model* is a statistical model associating the joint distribution of a random vector $X = (X_1, \ldots, X_p)$ to a graph $\mathcal{G}$. The graph describes the dependence structures possible within the graphical model: nodes of $\mathcal{G}$ represent entries of the random vector X and missing edges represent conditional independence constraints between corresponding the entries of X. The graphical view of a statistical model allows to study properties of the model by combining a graph theoretic analysis of the associated graph to probabilistic arguments.

A special type of graphical models that we study in this thesis are *Gaussian graphical models*. In a Gaussian graphical model, the random vector X follows a multivariate Normal distribution with covariance matrix Σ and mean μ. Since the interactions between the entries of X are fully specified by the covariance matrix, a Gaussian graphical model is a multivariate Normal model in which the covariance matrix Σ is constrained by the associated graph. Before being associated to graphs, multivariate Gaussian models with constraints on the covariance matrix have long been studied under the name of *covariance selection models* as introduced by Dempster [14].

When studying graphical models, one might naturally be interested in statistical questions related to the structure of the associated graph. Consider a graphical model $\mathcal{P}$ associated to a graph $\mathcal{G}$ and parametrized by a vector $\theta \in \Theta \subset \mathbb{R}^d$, that is, $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$. If $\mathcal{G}_0$ is a subgraph constructed by removing edges from $\mathcal{G}$, we call $\mathcal{P}_0 \subset \mathcal{P}$ the *submodel* of $\mathcal{P}$ associated to $\mathcal{G}_0$ and we have that $\mathcal{P}_0 = \{P_\theta : \theta \in \Theta_0\}$ with $\Theta_0 \subset \Theta$. In this thesis, we will be interested in testing statistical hypothesis of the form

$$H_0 : \theta \in \Theta_0 \quad \text{vs.} \quad H_1 : \theta \in \Theta \setminus \Theta_0.$$

That is, we are interested in knowing whether the true graphical model is associated to the sub-graph $\mathcal{G}_0$.

A standard approach for testing such a problem is the likelihood ratio test. The likelihood

ratio test provides a generic approach that can be applied in a wide variety of models, based on the difference in maximum log-likelihood attainable in each model. Assuming that the null hypothesis H_0 is true and under mild conditions, it can be shown that the likelihood ratio statistic converges to a χ^2_d distribution, where d is the number of restrictions imposed by H_0. This generic result has led to a large adoption of this method in many statistical settings. However, it was recognized early-on that the χ^2_d approximation might not work well in finite sample and can be vastly improved by considering corrected versions of the likelihood ratio statistics. In an influential paper [5], Bartlett shows that the likelihood ratio could be adjusted with a multiplicative factor to improve the accuracy of the χ^2_d approximation. Later, similar methods exploiting higher-order expansions of the characteristic function were developed under the term of *higher-order statistics* to construct asymptotic approximations and adjustments to statistics which are highly accurate in small samples. Barndorff-Nielsen and Cox [4, 12] offer a wide overview of the development and application of such methods.

In this thesis, we are interested in studying applications of higher-order approximations for testing subgraph null hypotheses of Gaussian graphical models. Eriksen [16] shows that the χ^2_d approximation behaves very poorly in small samples and proposes an alternative test statistic based on a transformation of the likelihood ratio for which accurate higher-order approximations can be derived. We present the work of Eriksen and empirically show that it can be employed in a setting where the dimension of the problem grows with the sample size.

We structure the thesis as follows. In Chapter 2, we provide an introduction to higher-order approximation methods and present multi-dimensional convergence proofs based on the modern material from Kolassa [20]. In Chapter 3, we bring our attention to Gaussian graphical models and present selected results concerning the existence of the maximum likelihood estimator based on Uhler [23, Chapter 9]. We then apply higher-order methods to submodel selection in Gaussian graphial models following the work of Eriksen [16]. Finally, we numerically study the behaviour of Eriksen's test statistic in a setting where the dimension of the problem is large compared to the sample size.

The source code for the approximations developed in this thesis are made available online[1], alongside with the code to reproduce the figures and various experiments presented.

[1] https://github.com/matthieubulte/masterthesis/tree/master/code

2 Higher-order statistics

This chapter introduces the necessary theoretical tools to construct and study higher-order statistics. In Section 2.1, we review the role and some properties of the characteristic function to study continuous multivariate distributions. In Section 2.2, we show how these results can be used to construct the Edgeworth approximation to the density of a standardized sum of i.i.d. random variables. We then study the convergence of this approximation scheme and illustrate theoretical results by applying it to simple distributions. In Section 2.5, we present the Saddlepoint approximation and compare it to the Edgeworth approximation. We demonstrate how this approximation can be used to approximate the density of the maximum likelihood estimator in an exponential family, linking the Saddlepoint approximation to the p^* approximation. We conclude this chapter with a numerical comparison of the p^* approximation and the standard Normal approximation to the density of the maximum likelihood estimator.

2.1 The characteristic function and related quantities

The *characteristic function* is a central tool in studying probability distributions. In this section, we review general results about the characteristic function of a multivariate continuous random variable. Let $p \in \mathbb{N}$ and let X be a random vector in $\mathbb{R}^p$. The characteristic function of X is the function $\zeta : \mathbb{R}^p \to \mathbb{C}$ given by

$$\zeta(t) = \mathbb{E}\left[\exp\left(it^\top X\right)\right].$$

The characteristic function is an essential tool in studying distributions. Indeed, the following multidimensional extension of [20, Theorem 2.4.2] shows that, under regularity conditions on the characteristic function, the density of a random vector exists and can be expressed in terms of the characteristic function.

Theorem 2.1. Let $X \sim P$ be a random vector in $\mathbb{R}^p$ with characteristic function $\zeta \in L^1(\mathbb{R}^p)$. Then, the density of X exists and is given by

$$f(x) = (2\pi)^{-p} \int_{\mathbb{R}^p} \exp\left(-it^\top x\right) \zeta(t) \mathrm{d}t. \tag{2.1}$$

Proof. Let $A \subset \mathbb{R}^p$ be a bounded rectangle $A = [a_1, b_1] \times \ldots \times [a_p, b_p]$ with $P(X \in \partial A) = 0$.

By Theorem 3.10.4 in [15], we have that

$$P(X \in A) = \lim_{T\to\infty} (2\pi)^{-p} \int_{[-T,T]^p} \zeta(t) \prod_{k=1}^{p} \frac{\exp(-it_k a_k) - \exp(-it_k b_k)}{it_k} \mathrm{d}t.$$

By rewriting various terms under the integral, one obtains

$$\begin{aligned} P(X \in A) &= \lim_{T\to\infty} (2\pi)^{-p} \int_{[-T,T]^p} \zeta(t) \prod_{k=1}^{p} \frac{\exp(-it_k a_k) - \exp(-it_k b_k)}{it_k} \mathrm{d}t \\ &= \lim_{T\to\infty} (2\pi)^{-p} \int_{[-T,T]^p} \zeta(t) \prod_{k=1}^{p} \int_{a_k}^{b_k} \exp(-it_k x_k)\, \mathrm{d}x_k \mathrm{d}t \\ &= \lim_{T\to\infty} (2\pi)^{-p} \int_{[-T,T]^p} \zeta(t) \int_A \exp\left(-it^\top x\right) \mathrm{d}x \mathrm{d}t. \end{aligned}$$

Since $\zeta \in L^1(\mathbb{R}^p)$ and A is bounded, the integrand in the previous equation is integrable, and the limit $T \to \infty$ can be replaced by the proper integral over $\mathbb{R}^p$. Further, using the absolute convergence property of ζ, Fubini's Theorem allows us to change the order of integration, which gives us

$$\begin{aligned} P(X \in A) &= (2\pi)^{-p} \int_{\mathbb{R}^p} \int_A \zeta(t) \exp\left(-it^\top x\right) \mathrm{d}x \mathrm{d}t \\ &= \int_A (2\pi)^{-p} \int_{\mathbb{R}^p} \zeta(t) \exp\left(-it^\top x\right) \mathrm{d}t \mathrm{d}x. \end{aligned}$$

By definition, this shows that the density of X exists and is given by (2.1). □

If X has a density function, the characteristic function of X corresponds to the *Fourier transform* of its density. Taking this generalized view of characteristic functions allows us to study approximations of densities that are not necessarily densities and characteristic functions themselves. We employ a less commonly used definition of the Fourier transform, in which the sign of the exponent is reversed. For $f \in L^1(\mathbb{R}^p)$, the Fourier transform $\mathcal{F}[f]$ of f is the function given by

$$\mathcal{F}[f](t) = \int_{\mathbb{R}^p} \exp\left(it^\top x\right) f(x) \mathrm{d}x \qquad \text{for all } t \in \mathbb{R}^p. \tag{2.2}$$

In this context, we generalize Theorem 2.1 to provide the necessary conditions under which the Fourier transform can be inverted. This extends [20, Corollary 2.4.3] to $\mathbb{R}^p$.

Corollary 2.2. Suppose that $f \in L^1(\mathbb{R}^p)$ and $\zeta \in L^1(\mathbb{R}^p)$ are related by

$$\zeta(t) = \mathcal{F}[f](t) \qquad \text{for all } t \in \mathbb{R}^p. \tag{2.3}$$

Then, for any $x \in \mathbb{R}^p$, it holds that

$$f(x) = (2\pi)^{-p} \int_{\mathbb{R}^p} \exp\left(-it^\top x\right) \zeta(t) \mathrm{d}t. \tag{2.4}$$

Proof. We decompose f in positive and negative parts by $f(x) = f^+(x) - f^-(x)$ where $f^+(x) = f(x)\mathbb{1}_{f(x)\geq 0}$ and $f^-(x) = -f(x)\mathbb{1}_{f(x)<0}$. Then, if $c^+ = \int_{\mathbb{R}^p} f^+(x)\mathrm{d}x$ and $c^- = \int_{\mathbb{R}^p} f^-(x)\mathrm{d}x$, the functions f^+/c^+ and f^-/c^- are both densities over $\mathbb{R}^p$ with respective characteristic functions ζ^+ and ζ^-. By replacing these quantities in (2.3), it follows that

$$\begin{aligned}
\zeta(t) &= \int_{\mathbb{R}^p} \exp\left(it^\top x\right) f(x)\mathrm{d}x \\
&= c^+ \int_{\mathbb{R}^p} \exp\left(it^\top x\right) \frac{1}{c^+} f^+(x)\mathrm{d}x - c^- \int_{\mathbb{R}^p} \exp\left(it^\top x\right) \frac{1}{c^-} f^-(x)\mathrm{d}x \\
&= c^+\zeta^+(t) - c^-\zeta^-(t).
\end{aligned}$$

Since $\zeta \in L^1(\mathbb{R}^p)$, we have that $\zeta^\pm \in L^1(\mathbb{R}^p)$ and the conditions of Theorem 2.1 are satisfied by ζ^+ and ζ^-. We then obtain that

$$\frac{1}{c^\pm} f^\pm(x) = (2\pi)^{-p} \int_{\mathbb{R}^p} \exp\left(-it^\top x\right) \zeta^\pm(t)\mathrm{d}t.$$

Hence

$$\begin{aligned}
f(x) &= f^+(x) - f^-(x) \\
&= c^+ (2\pi)^{-p} \int_{\mathbb{R}^p} \exp\left(-it^\top x\right) \zeta^+(t)\mathrm{d}t - c^- (2\pi)^{-p} \int_{\mathbb{R}^p} \exp\left(-it^\top x\right) \zeta^-(t)\mathrm{d}t \\
&= (2\pi)^{-p} \int_{\mathbb{R}^p} \exp\left(-it^\top x\right) \left[c^+\zeta^+(t) - c^-\zeta^-(t)\right] \mathrm{d}t \\
&= (2\pi)^{-p} \int_{\mathbb{R}^p} \exp\left(-it^\top x\right) \zeta(t)\mathrm{d}t.
\end{aligned}$$

□

This corollary lets us extend the notation introduced in (2.2) and define the inverse Fourier transform operator $\mathcal{F}^{-1}[\zeta]$ of $\zeta \in L^1(\mathbb{R}^p)$ as in (2.4), defined for every $x \in \mathbb{R}^p$ by

$$\mathcal{F}^{-1}[\zeta](x) = (2\pi)^{-p} \int_{\mathbb{R}^p} \exp\left(-it^\top x\right) \zeta(t)\mathrm{d}t.$$

In order to better understand the characteristic function, we need to be able to know in which functional space it lies in. The following lemma relates L^p integrability of the characteristic function to the existence of the density of a convolution of random variables. This is an extension of [20, Lemma 2.4.4] to $\mathbb{R}^p$.

Lemma 2.3. The characteristic function ζ of a random variable X in $\mathbb{R}^p$ satisfies $\zeta \in L^q(\mathbb{R}^p)$ for some $q > 1$ if and only if there exists a positive integer $l \in \mathbb{N}$ such that the density of a convolution of l independent copies of X exists and is bounded.

Proof. The *only if* direction is a direct consequence of Theorem 2.1. Assuming that $\zeta \in L^q(\mathbb{R}^p)$ we have that $\zeta \in L^l(\mathbb{R}^p)$ for $l = \lceil q \rceil$ and hence,

$$\int_{\mathbb{R}^p} \left|\zeta(t)^l\right| \mathrm{d}t < \infty.$$

Thus, $\zeta^l \in L^1(\mathbb{R}^p)$. Since the characteristic function of a sum of l independent copies of X is equal to $t \mapsto \zeta(t)^l$, we can apply Theorem 2.1. This shows that the density of the convolution of l copies of X exists and is bounded.
We now prove the *if* direction of the lemma. Assume that there exists a positive interger $j \in \mathbb{N}$ such that the density f_j of a convolution of j independent copies of X exists and is bounded. Then, using that $|\zeta(-t)| = \left|\overline{\zeta(t)}\right| = |\zeta(t)|$, we have that for any $r \in \mathbb{R}$,

$$\int_{[-r,r]^p} |\zeta(t)|^{2j} \mathrm{d}t = \int_{[-r,r]^p} |\zeta(t)|^j |\zeta(t)|^j \mathrm{d}t = \int_{[-r,r]^p} |\zeta(t)|^j |\zeta(-t)|^j \mathrm{d}t.$$

Furthermore, by the definition of the characteristic function and using Fubini's theorem, we have that

$$\begin{aligned}\int_{[-r,r]^p} |\zeta(t)|^{2j} \mathrm{d}t &= \int_{[-r,r]^p} \left[\int_{\mathbb{R}^p} f_j(x) \exp\left(it^\top x\right) \mathrm{d}x\right] \left[\int_{\mathbb{R}^p} f_j(y) \exp\left(-it^\top y\right) \mathrm{d}y\right] \mathrm{d}t \\ &= \int_{\mathbb{R}^p} \int_{\mathbb{R}^p} \int_{[-r,r]^p} f_j(x) f_j(y) \exp\left(it^\top (x-y)\right) \mathrm{d}t \mathrm{d}y \mathrm{d}x.\end{aligned}$$

Setting $z = y - x$ and using the identity $\sin x = (\exp(ix) - \exp(-ix))/2i$, we get

$$\begin{aligned}
\int_{[-r,r]^p} |\zeta(t)|^{2j} \,\mathrm{d}t &= \int_{\mathbb{R}^p} \int_{\mathbb{R}^p} \int_{[-r,r]^p} f_j(x) f_j(x+z) \exp\left(-it^\top z\right) \mathrm{d}t \mathrm{d}z \mathrm{d}x \\
&= \int_{\mathbb{R}^p} \int_{\mathbb{R}^p} f_j(x) f_j(x+z) \left[\prod_{k=1}^p \int_{[-r,r]} \exp\left(-it^\top z_k\right)\right] \mathrm{d}t \mathrm{d}z \mathrm{d}x \\
&= \int_{\mathbb{R}^p} \int_{\mathbb{R}^p} f_j(x) f_j(x+z) \left[\prod_{k=1}^p \frac{\exp(-irz_k) - \exp(irz_k)}{-iz_k}\right] \mathrm{d}z \mathrm{d}x \\
&= \int_{\mathbb{R}^p} \int_{\mathbb{R}^p} f_j(x) f_j(x+z) \left[\prod_{k=1}^p \frac{2\sin(rz_k)}{z_k}\right] \mathrm{d}z \mathrm{d}x.
\end{aligned}$$

Applying the change of variable $v = rz$ gives us

$$\begin{aligned}
\int_{[-r,r]^p} |\zeta(t)|^{2j} \,\mathrm{d}t &= \int_{\mathbb{R}^p} \int_{\mathbb{R}^p} f_j(x) f_j(x+v/r) \left[\prod_{k=1}^p \frac{2\sin(v_k)}{v_k/r}\right] r^{-p} \mathrm{d}v \mathrm{d}x \\
&= \int_{\mathbb{R}^p} \int_{\mathbb{R}^p} f_j(x) f_j(x+v/r) \left[\prod_{k=1}^p \frac{2\sin(v_k)}{v_k}\right] \mathrm{d}v \mathrm{d}x.
\end{aligned}$$

Using the fact that $\sup_{x\in\mathbb{R}} |\sin x/x| < 1$, we have that $\prod_{k=1}^p \frac{2\sin(v_k)}{v_k} < 2^p$ and

$$\int_{[-r,r]^p} |\zeta(t)|^{2j} \,\mathrm{d}t \leq 2^p \int_{\mathbb{R}^p} f_j(x) \int_{\mathbb{R}^p} f_j(x+v/r) \mathrm{d}v \mathrm{d}x = 2^p \int_{\mathbb{R}^p} f_j(x) \mathrm{d}x = 2^p.$$

This shows that a finite upper bound on $\|\zeta\|_{2j}^{2j}$ exists, that is independent of r. This concludes the proof for $q = 2j$. □

In the following sections, we study approximations of the characteristic function in terms of its Taylor approximation. As one might expect, computing the Fourier and inverse Fourier transforms of such approximations involves computing the Fourier transform of derivatives of the characteristic function. Before studying Fourier transforms of differential quantities, we introduce some notation for multivariate derivatives.

For $k \in \mathbb{N}$, we define $S_p(k)$ as the set of index tuples of length k over p-dimensional vectors, that is,

$$S_p(k) = \{(s_1, \ldots, s_k) : s_i \in [p]\},$$

where $[p] = \{1, \ldots, p\}$. Let $f : \mathbb{R}^p \to \mathbb{R}$ be a k-times differentiable function, let $s \in S_p(k)$

and let $x_0 \in \mathbb{R}^p$. Then the *s-derivative* of f in x_0 is given by

$$D^s f(x_0) = \frac{\mathrm{d}^k}{\mathrm{d}x_{s_1} \dots \mathrm{d}x_{s_k}} f(x)\bigg|_{x=x_0}.$$

We now proceed to the following lemma, which gives a simple expression of the Fourier transform of derivatives of a function.

Lemma 2.4. Let $k \in \mathbb{N}$ and $f \in L^1(\mathbb{R}^p)$ such that all partial derivatives of f of order up to k exist, and for any $\tilde{s} \in S_p(k-1)$,

$$\lim_{\|x\| \to \infty} \exp\left(it^\top x\right) D^{\tilde{s}} f(x) = 0. \tag{2.5}$$

Then for any $s \in S_p(k)$, it holds that

$$\mathcal{F}\left[D^s f\right](t) = (-i)^k t^s \mathcal{F}[f].$$

Proof. Let $\tilde{s} = (s_1, \dots, s_{k-1})$, then by direct computation of the Fourier transform,

$$\begin{aligned}
\mathcal{F}\left[D^s f\right](t) &= (2\pi)^{-p} \int_{\mathbb{R}^p} \exp\left(it^\top x\right) D^s f(x) \mathrm{d}x \\
&= (2\pi)^{-p} \int_{\mathbb{R}^{-1}} \int_{\mathbb{R}} \exp\left(it^\top x\right) \frac{\mathrm{d}}{\mathrm{d}x_{s_k}} D^{\tilde{s}} f(x) \mathrm{d}x_{s_k} \mathrm{d}x_{\tilde{s}}\,.
\end{aligned}$$

Integrating by part over the axis x_{s_k} and using Assumption (2.5) gives,

$$\begin{aligned}
\mathcal{F}\left[D^s f\right](t) &= -(2\pi)^{-p} \int_{\mathbb{R}^p} (it_{s_k}) \exp\left(it^\top x\right) D^{\tilde{s}} f(x) \mathrm{d}x \\
&= -it_{s_k} (2\pi)^{-p} \int_{\mathbb{R}^p} \exp\left(it^\top x\right) D^{\tilde{s}} f(x) \mathrm{d}x \\
&= -it_{s_k} \mathcal{F}\left[D^{\tilde{s}} f\right](t)
\end{aligned}$$

Iterating the previous steps completes the proof. □

Next, we introduce the *cumulant generating function*, a quantity related to the characteristic function relevant to the construction of density approximations. For a random vector X in $\mathbb{R}^p$, the cumulant generating function of X is the function $K : \mathbb{R}^p \to \mathbb{R}$ given by

$$K(t) = \log \mathbb{E}\left[\exp\left(t^\top X\right)\right].$$

The derivatives of the cumulant generating function are called the *cumulants*. Let $s \in$

$S_p(k)$ be an index vector of length $k \in \mathbb{N}$, then if the involved derivatives exist, we define the *s-cumulant* of X as

$$\kappa_s(X) = D^s K(0).$$

In the sequel, cumulants might depend on various quantities such as the sample size, the random variable of interest or parameters of a distribution, in which case we will use variations of the notation κ_s to make clear which cumulants are being discussed.

Since the Normal distribution will often be used in the sequel, the next example gives the cumulant generating function and cumulants of a multivariate Normal distribution.

Example 2.5. Let $X \sim N(\mu, \Sigma)$ with $\mu \in \mathbb{R}^p$ and $\Sigma \in \mathcal{S}_p$. The cumulant generating function $K(t; \mu, \Sigma)$ of X is the quadratic function given by

$$K(t; \mu, \Sigma) = t^\top \mu + t^\top \Sigma t.$$

Since K is quadratic in t, it is clear that cumulants of X of arbitrary order exist. Furthermore, the first order cumulants are the components μ, the second order cumulants are the components of Σ, and the cumulants of order higher than 2 are equal to 0.

We now state, without a proof, some simple properties of cumulants that will be useful in future proofs.

Lemma 2.6. Let $X_1, \ldots, X_n \overset{iid}{\sim} P$. Then the following holds for any $s \in S(k)$

i. $\kappa_s(X_1 + \ldots + X_n) = n\kappa_s(X_1)$

ii. For all $c \in \mathbb{R}$, $\kappa_s(cX_1) = c^k \kappa_s(X_1)$

iii. For all $c \in \mathbb{R}^p$, $\kappa_s(X_1 + c) = \begin{cases} \kappa_s(X_1) + c_i & \text{if } s = (i), \\ \kappa_s(X_1) & \text{otherwise,} \end{cases}$

where we write $\kappa_s(Z)$ for the s-cumulant of the random variable Z.

Note that the cumulant generating function is closely related to the characteristic function since

$$K(t) = \log \mathbb{E}\left[\exp\left(t^\top X\right)\right] = \log \mathbb{E}\left[\exp\left(i(-i)t^\top X\right)\right] = \log \zeta(-it).$$

This equality allows us to define the cumulants $\kappa_s(X)$ for $s \in S_p(k)$ in terms of the

characteristic function

$$\kappa_s(X) = D^s K(0) = \frac{\mathrm{d}^k}{\mathrm{d}x_{s_1} \dots \mathrm{d}x_{s_k}} \log \zeta(-it)\bigg|_{t=0} = (-i)^k D^s \log \zeta(0),$$

and hence

$$D^s \log \zeta(0) = i^k \kappa_s(X).$$

2.2 Heuristic introduction to the Edgeworth approximation

We now present a heuristic development of the Edgeworth approximation [**?**]. Consider two distributions P and Q over $\mathbb{R}^p$ with respective densities f and q, characteristic functions ζ and ξ, and cumulants κ_s and γ_s for $s \in S_p(k)$, $k \in \mathbb{N}$. Assume that both P and Q have mean 0 and a covariance matrix equal to $\mathbb{1}_p$. We wish to utilize the cumulants of both distributions to construct an approximation of the density of P.

By formal expansion of the difference between the cumulant generating functions of P and Q around 0, we obtain that for any $t \in \mathbb{R}^p$,

$$\begin{aligned} \log \frac{\zeta(t)}{\xi(t)} = \log \zeta(t) - \log \xi(t) &= \sum_{r=0}^{\infty} \sum_{s \in S_p(r)} (\kappa_s - \gamma_s) \frac{i^r t^s}{r!} \\ &= \sum_{r=3}^{\infty} \sum_{s \in S_p(r)} (\kappa_s - \gamma_s) \frac{i^r t^s}{r!}, \end{aligned}$$

where the last equality follows from the assumption of shared mean and covariance of P and Q. Exponentiating on both sides of the equation and isolating $\zeta(t)$, we find that

$$\zeta(t) = \xi(t) \exp\left\{ \sum_{r=3}^{\infty} \sum_{s \in S_p(r)} (\kappa_s - \gamma_s) \frac{i^r t^s}{r!} \right\}.$$

Let $\alpha_s = \kappa_s - \gamma_s$. By taking a formal expansion of the exponential function, we have that

$$\begin{aligned}\zeta(t) &= \xi(t) \exp\left\{\sum_{r=3}^{\infty} \sum_{s \in S_p(r)} \alpha_s \frac{i^r t^s}{r!}\right\} \\ &= \xi(t) \sum_{j=0}^{\infty} \frac{1}{j!} \left\{\sum_{r=3}^{\infty} \sum_{s \in S_p(r)} \alpha_s \frac{i^r t^s}{r!}\right\}^j \\ &= \sum_{j=0}^{\infty} \frac{1}{j!} \sum_{\substack{r_1=3 \\ \dots \\ r_j=3}}^{\infty} \sum_{\substack{s_1 \in S_p(r_1) \\ \dots \\ s_j \in S_p(r_j)}} \alpha_{s_1} \dots \alpha_{s_j} \frac{\xi(t) i^{r_1+\dots+r_j} t^{s_1} \dots t^{s_j}}{r_1! \dots r_j!}.\end{aligned}$$

We can simplify the notation by replacing the summation over r_k and s_k by a sum over a single pair (r, s) and grouping together the coefficients of the power t^s. To do so, we introduce the *pseudo-cumulants* α_s^* satisfying

$$\zeta(t) = \sum_{j=0}^{\infty} \sum_{s \in S_p(j)} \alpha_s^* \frac{\xi(t) i^j t^s}{j!}. \tag{2.6}$$

One sees that for $s \in S_p(j)$, the pseudo-cumulant α_s^* is a sum over products of the form $\prod_{i=1}^{l} \alpha_{s_i}$ where $s_1 \in S_p(j_1), \dots, s_l \in S_p(j_l)$ such that $j_1 + \dots + j_l = j$, and such that the indices in s and $s_1, \dots, s_l$ match. For instance, for $j = 1, 2, 3$, the pseudo-cumulants are of the following form,

$$\begin{aligned} j = 1 : &\qquad \alpha^*_{(k)} = \alpha_{(k)} \\ j = 2 : &\qquad \alpha^*_{(k,l)} = \alpha_{(k,l)} + \alpha_{(k)}\alpha_{(l)} \\ j = 3 : &\qquad \alpha^*_{(k,l,m)} = \alpha_{(k,l,m)} + \alpha_{(k,l)}\alpha_{(m)} + \alpha_{(k)}\alpha_{(l)}\alpha_{(m)}, \end{aligned}$$

where $k, l, m \in [p]$ and the exact coefficient in front of the α terms are not relevant and ignored for conciseness. Now, assuming that the conditions of Lemma 2.4 are satisfied by the density q of Q, we recognize that

$$\xi(t)(-i)^j t^s = \mathcal{F}\left[D^s q\right].$$

This allows us to retrieve the density of P by Fourier inversion,

$$f(x) = \mathcal{F}^{-1}[\zeta] = \sum_{j=0}^{\infty} \sum_{s \in S_p(j)} \alpha_s^* \frac{(-1)^j D^s q(x)}{j!}$$
$$= q(x) \left\{ 1 + \sum_{j=1}^{\infty} \sum_{s \in S_p(j)} \alpha_s^* \frac{(-1)^j D^s q(x)}{j! q(x)} \right\}. \tag{2.7}$$

A convenient choice for Q is the multivariate standard Normal distribution $\mathcal{N}_p(0, \mathbb{1}_p)$ with density $\phi : \mathbb{R}^p \to \mathbb{R}$. In this case, the cumulants of P and Q of order $k = 1, 2$ of the two distributions match, implying that $\alpha_s = 0$ for any $s \in S_p(k)$ and $k = 1, 2$. Since the pseudo-cumulants α^* are composed of sums and products of the coefficients α, this also implies that the pseudo-cumulants of order $k = 1, 2$ are 0 as well. Using this in (2.7), we obtain that

$$f(x) = \phi(x) \left\{ 1 + \sum_{j=3}^{\infty} \sum_{s \in S_p(j)} \alpha_s^* \frac{(-1)^j D^s \phi(x)}{j! \phi(x)} \right\}$$
$$= \phi(x) \left\{ 1 + \sum_{j=3}^{\infty} \sum_{s \in S_p(j)} \frac{1}{j!} \alpha_s^* h_s(x) \right\}, \tag{2.8}$$

where $h_s(\cdot)$ are a multivariate generalization of the Hermite polynomials, given by

$$h_s(x) = (-1)^j \frac{D^s \phi(x)}{\phi(x)}. \tag{2.9}$$

Next, we apply this transformation to the standardized sum $Y = n^{-1/2} \sum_{i=1}^n X_i$ where $X_1, \ldots, X_n$ are i.i.d. copies of $X \sim P$. For any $s \in S_p(k)$, using properties (i) and (ii) of cumulants given in Lemma 2.6, the s-cumulants of Y are given by

$$\kappa_s(Y) = n^{1-k/2} \kappa_s(X) = O(n^{1-k/2}).$$

We can form the *Edgeworth approximation* of order k, denoted $e_{k,n}(\cdot; \kappa(X))$, by only keeping cumulants of order up to k and removing terms of order $o(n^{1-k/2})$ in (2.8). The notation $e_{k,n}(\cdot; \kappa(X))$ highlights the fact that the approximation to the density of Y only depends on three parameters: the order k, the number of terms summed n, and the cumulants $\kappa(X)$ of the summands. Since we discard all cumulants of order higher than k, the error of the resulting approximation must be at least $O(n^{(1-k)/2})$ and we have

$$f_Y(y) = e_{k,n}(y; \kappa(X)) + o(n^{1-k/2}), \tag{2.10}$$

Note that this equation can be slightly refined, which will be of use in the sequel. After truncating (2.8), the density f can be decomposed as follows

$$f(y) = \phi(y)\left\{1 + P_{k,n}(y; \kappa(X)) + o(n^{1-k/2})\right\}, \tag{2.11}$$

where $P_{k,n}(\cdot; \kappa(X))$ is the polynomial part of the Edgeworth approximation.

Example 2.7. Consider a random variable $X \in \mathbb{R}$ with cumulants $\kappa(X) = (\kappa_{(1)}, \kappa_{(2)}, \ldots)$ such that $\mathbb{E}X = 0$ and $\mathbb{V}[X] = 1$. In one dimension, (2.8) becomes

$$f(x) = \phi(x)\left\{1 + \sum_{j=3}^{\infty} \frac{1}{j!}\alpha_j^* h_j(x)\right\}.$$

Let Y be a standardized sum of n independent copies of X. To construct the Edgeworth approximation of order $k = 4$ of the density of Y, we truncate the above equation to only keep cumulants of order up to 4: $\kappa_{(3)}$ and $\kappa_{(4)}$. As mentioned ealier, each cumulant $\kappa_{(k)}(Y)$ is of order $O(n^{1-k/2})$, hence, the following products of cumulants can result in a term of the desired orders

$$\kappa_{(3)}(Y) = \frac{\kappa_{(3)}}{\sqrt{n}} \qquad \kappa_{(3)}(Y)\kappa_{(3)}(Y) = \frac{\kappa_{(3)}^2}{n} \qquad \kappa_{(4)}(Y) = \frac{\kappa_{(4)}}{n}.$$

Finding the right coefficients of each of these terms from the definition of the corresponding α^*, we obtain the following expression of the Edgeworth approximation

$$e_{4,n}(y; \kappa(X)) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{y^2}{2}\right)\left\{1 + \frac{\kappa_{(3)}H_3(y)}{6\sqrt{n}} + \frac{3\kappa_{(4)}H_4(y) + \kappa_{(3)}^2 H_6(y)}{72n}\right\}. \tag{2.12}$$

While the argument provided above for the definition of the Edgeworth series is not sufficiently rigorous to prove (2.10), we now show that the Edgeworth series $e_{k,n}(y; \kappa(X))$ indeed approximates the density of a standardized sum with an error of $o(n^{1-k/2})$.

Remark 2.8. The initial assumption of having mean 0 and a covariance matrix equal to the identity does not imply a loss of generality of the approach. Indeed, if X has a mean μ and covariance matrix Σ, the Edgeworth series $e_{k,n}(\cdot; \kappa(Z))$ can be constructed for the standardized random variable $Z = \Sigma^{-1/2}(X - \mu)$ and can be used to construct an approximation $e_{k,n}(\cdot; \kappa(X))$ of the density of $n^{-1/2}\sum_{i=1}^n X_i$ by applying the corresponding

change of variable formula, giving

$$e_{k,n}(s;\kappa(X)) = |\Sigma|^{-1/2}\, e_{k,n}(\Sigma^{-1/2}(s-\sqrt{n}\mu);\kappa(Z)).$$

In the sequel, we use the Edgeworth expansion to approximate the density of random variables which are not necessarily centered or have a unit covariance. In this case, we implicitly make use of the change of variable formula mentioned in the following remark.

Remark 2.9. Note that one can show from the definition of generalized Hermite polynomials in (2.9), that for any index tuple $s \in S_p(k)$, where $k \in \mathbb{N}$ is an odd integer, 0 is a root of the generalized Hermite polynomial h_s. Furthermore, by the development of (2.8), the coefficient of each Hermite polynomial h_s, where $s \in S_p(k)$, contains terms of order $O(n^{1-k'/2})$ where k and k' have the same parity and $k' \leq k$.

Combining this with Remark 2.8 shows that the polynomial part of the Edgeworth series evaluated at the mean of the approximated distribution is a polynomial in n^{-1} instead of a polynomial in $n^{-1/2}$ since terms of odd powers are zero. Another consequence of this is that the error at the mean of the Edgeworth approximation of even order k is $O(n^{-k/2})$.

For instance, if $e_{4,n}(\cdot;\kappa(X))$ is the Edgeworth expansion of order 4 from Example 2.7, we have that

$$f_Y(y) = e_{4,n}(y;\kappa(X)) + \begin{cases} O(n^{-2}) & \text{if } y = 0, \\ o(n^{-1}) & \text{otherwise.} \end{cases}$$

2.3 Convergence of the Edgeworth approximation

While the previous section provided an intuition for the development of the Edgeworth approximation, it is not a rigorous proof. In this section, we develop a proof for the convergence claim in (2.10).

Recall that in the first step of the development of the Edgeworth approximation, the ratio of characteristic functions ζ/ξ is approximated via two truncated Taylor expansions,

$$\begin{array}{ccccccc} \log\zeta(t) - \log\xi(t) = & u & \longrightarrow & \exp u & = & \zeta(t)/\xi(t) \\ & \approx & & \approx & & \approx \\ & v & \longrightarrow & \sum_{k=0}^{l} v^k/k! & = & z \end{array}$$

The following lemma from [20, Theorem 2.5.3] bounds the error found in approximating $\exp u$ by the truncated Taylor expansion of $\exp(\cdot)$ evaluated at a point v near u.

Lemma 2.10. Let $u, v \in \mathbb{C}$ and $l \in \mathbb{N}$, then the following inequality holds,

$$\left|\exp u - \sum_{k=0}^{l} \frac{v^k}{k!}\right| \leq \max\left\{\exp|u|, \exp|v|\right\} \left(|u-v| + \left|\frac{v^{l+1}}{(l+1)!}\right|\right). \tag{2.13}$$

Proof. By the triangle inequality,

$$\left|\exp u - \sum_{k=0}^{l} \frac{v^k}{k!}\right| \leq |\exp u - \exp v| + \left|\sum_{k=l+1}^{\infty} \frac{v^k}{k!}\right|.$$

We begin by upper bounding the second term on the right hand side as follows,

$$\begin{aligned}
\left|\sum_{k=l+1}^{\infty} \frac{v^k}{k!}\right| &\leq \sum_{k=l+1}^{\infty} \left|\frac{v^k}{k!}\right| = \left|\frac{v^{l+1}}{(l+1)!}\right| \sum_{k=0}^{\infty} |v^k| \frac{(l+1)!}{(k+l+1)!} \\
&\leq \left|\frac{v^{l+1}}{(l+1)!}\right| \sum_{k=0}^{\infty} \left|\frac{v^k}{k!}\right| = \left|\frac{v^{l+1}}{(l+1)!}\right| \exp v \\
&\leq \left|\frac{v^{l+1}}{(l+1)!}\right| \max\left\{\exp|u|, \exp|v|\right\}.
\end{aligned}$$

Furthermore, by Taylor's theorem, there exists $\theta \in (0,1)$ such that for $z = \theta u + (1-\theta)v$

$$|\exp u - \exp v| = |u - v| \exp z.$$

Using the convexity of the exponential function, we find the following bound

$$|\exp u - \exp v| \leq |u - v| \max\left\{\exp|u|, \exp|v|\right\}.$$

Combining the above two bounds completes the proof of the lemma. □

Continuing the development of the Edgeworth approximation, a pseudo-characteristic function was constructed based on the approximation of the ratio ζ/ξ. In the following theorem, we use the previous lemma and properties of cumulants to provide an asymptotic bound on the error obtained when using this approximation on the characteristic function of a standardized sum of random variables. This theorem is a specialization of [20, Corollary 2.5.4].

Theorem 2.11. Let ζ be the characteristic function of a random vector $X \in \mathbb{R}^p$ and let $n, k \in \mathbb{N}$. Assume that all cumulants of X of order up to k exist and that the second

cumulants of X satisfy $\kappa_{(i,j)} = \delta_{ij}$ for all $i, j \in [p]$. Let

$$\xi(t) = \exp\left(-\frac{1}{2}\|t\|_2^2\right) \sum_{l=0}^{k-2} \frac{1}{l!} \left[1 + \sum_{m=3}^{k} \sum_{s \in S_p(m)} \frac{i^m \kappa_s t^s}{n^{m/2-1} m!}\right]^l . \tag{2.14}$$

Then for every $\epsilon > 0$ there exists $\delta > 0$ and a constant $C_p > 0$ dependent on the dimension of X such that

$$\left|\zeta(tn^{-1/2})^n - \xi(t)\right| \leq \exp\left(-\frac{1}{4}\|t\|_2^2\right) \left[\frac{\epsilon \|t\|_2^k}{n^{k/2-1}} + \frac{C_p^{k-1} \|t\|_2^{3(k-1)}}{(k-1)! n^{k/2-1/2}}\right] \tag{2.15}$$

holds for all $t \in \mathbb{R}^p$ with $\|t\|_2 < \delta\sqrt{n}$.

Proof. The idea of this proof is to rewrite the left hand side of (2.15) to be able to use Lemma 2.10 and find suitable upper bounds on the remaining quantities. To that end, we define the functions $u(t) = nu^*(tn^{-1/2})$ and $v(t) = nv^*(tn^{-1/2})$, where

$$u^*(t) = \log \zeta(t) + \frac{1}{2}\|t\|_2^2$$

and

$$v^*(t) = \sum_{m=3}^{k} \sum_{s \in S_p(m)} \frac{i^m \kappa_s t^s}{m!}.$$

We then rewrite $\zeta(tn^{-1/2})^n$ as follows,

$$\zeta(tn^{-1/2})^n = \exp\left(n\left[\log \zeta(tn^{-1/2})\right]\right) = \exp\left(-\frac{1}{2}\|t\|_2^2\right) \exp u(t)$$

and

$$\xi(t) = \exp\left(-\frac{1}{2}\|t\|_2^2\right) \sum_{l=0}^{k-2} \frac{v(t)^l}{l!}.$$

Lemma 2.10 gives a bound on the left hand side of (2.15), and thus

$$\begin{aligned}
&\left|\zeta(tn^{-1/2})^n - \xi(t)\right| = \exp\left(-\frac{1}{2}\|t\|_2^2\right) \left|\exp u(t) - \sum_{l=0}^{k-2} \frac{v(t)^l}{l!}\right| \\
&\leq \exp\left(-\frac{1}{2}\|t\|_2^2\right) \max\left\{\exp|u(t)|, \exp|v(t)|\right\} \left(|u(t) - v(t)| + \frac{|v(t)|^{k-1}}{(k-1)!}\right)
\end{aligned}$$

Next, we find a suitable upper bound on the right hand side of the above inequality. First note that both u and v have continuous derivatives in 0 of order up to k. Starting with

u^*, let $s \in S_p(m)$ for $3 \leq m < k$, then

$$\begin{aligned} D^s u^*(0) &= \frac{\mathrm{d}}{\mathrm{d}t_{s_1}} \dots \frac{\mathrm{d}}{\mathrm{d}t_{s_m}} \log \zeta(t) + \frac{1}{2} \|t\|_2^2 \Big|_{t=0} \\ &= \frac{\mathrm{d}}{\mathrm{d}t_{s_1}} \dots \frac{\mathrm{d}}{\mathrm{d}t_{s_m}} \log \zeta(t) \Big|_{t=0} + \frac{\mathrm{d}}{\mathrm{d}t_{s_1}} \dots \frac{\mathrm{d}}{\mathrm{d}t_{s_m}} \frac{1}{2} \|t\|_2^2 \Big|_{t=0} \\ &= (-i)^{-m} \kappa_s = i^m \kappa_s, \end{aligned}$$

where the last equality follows from the fact that the derivative of $\|t\|_2^2$ is 0 since $\|t\|_2^2$ is quadratic in t and $|s| = m \geq 3$. Similarly, we can compute the derivatives of v^* in 0,

$$\begin{aligned} D^s v^*(0) &= \frac{\mathrm{d}}{\mathrm{d}t_{s_1}} \dots \frac{\mathrm{d}}{\mathrm{d}t_{s_m}} v^*(t) \Big|_{t=0} \\ &= \frac{\mathrm{d}}{\mathrm{d}t_{s_1}} \dots \frac{\mathrm{d}}{\mathrm{d}t_{s_m}} \sum_{m'=3}^{k} \sum_{s' \in S_p(m')} \frac{i^{m'} \kappa^{s'} t_{s'_1} \dots t_{s'_{m'}}}{m'!} \Big|_{t=0} \\ &= \sum_{m'=3}^{k} \sum_{s' \in S_p(m')} \frac{i^{m'} \kappa^{s'}}{m'!} \frac{\mathrm{d}}{\mathrm{d}t_{s_1}} \dots \frac{\mathrm{d}}{\mathrm{d}t_{s_m}} t_{s'_1} \dots t_{s'_{m'}} \Big|_{t=0}. \end{aligned}$$

Note that the term $\frac{\mathrm{d}}{\mathrm{d}t_{s_1}} \dots \frac{\mathrm{d}}{\mathrm{d}t_{s_m}} t_{s'_1} \dots t_{s'_{m'}}|_{t=0} = 1$ if and only if s' is a permutation of s, otherwise it is equal to 0. Hence

$$\frac{\mathrm{d}}{\mathrm{d}t_{s_1}} \dots \frac{\mathrm{d}}{\mathrm{d}t_{s_m}} v^*(t) \Big|_{t=0} = \sum_{s' \in S_p(m)} \frac{i^m \kappa^{s'}}{m!} = m! \frac{i^m \kappa^s}{m!} = i^m \kappa_s,$$

where the second equality holds as $\kappa_s = \kappa_{s'}$ for all permutation s' of s. Therefore all derivatives of order up to k of $u^* - v^*$ (and hence also $u - v$) exist in 0 and are all equal to 0. Thus, there exists $\delta > 0$ such that for all $t \in \mathbb{R}^p$ with $\|t\|_2 \leq \delta$,

$$|u^*(t) - v^*(t)| \leq \epsilon \|t\|_2^k .$$

If $\|t\|_2 \leq \delta\sqrt{n}$, this bound yields

$$|u(t) - v(t)| = n \left|u^*(tn^{-1/2}) - v(tn^{-1/2})\right| \leq n\epsilon \left\|n^{-1/2}t\right\|_2^k = n^{1-k/2} \|t\|_2^k \epsilon.$$

Now let $\delta > 0$ be small enough such that $|u^*(t)| < \|t\|_2^2 /4$ for $\|t\|_2 \leq \delta$. Then for $\|t\|_2 \leq \delta\sqrt{n}$ we have that

$$|u(t)| = n \left|u^*(tn^{-1/2})\right| \leq n \left\|tn^{-1/2}\right\|_2^2 /4 = \|t\|_2^2 /4.$$

We observe that all derivatives of v^* in 0 of first and second order are equal to 0 and that the third order derivatives of v^* are bounded. By Taylor's theorem, this allows us to find the following bound for all $\|t\|_2 \leq \delta\sqrt{n}$,

$$|v(t)| = |nv^*(tn^{-1/2})| < C_p n \left\|tn^{-1/2}\right\|_2^3 = C_p \|t\|_2^3 n^{-1/2},$$

where

$$C_p = \sup_{\substack{\|t\|_2 \leq \delta, \\ s \in S_p(3)}} p^3 \left|D^s v^*(t)\right|.$$

Hence, for $\delta > 0$ small enough and $t \leq \delta\sqrt{n}$, we have that

$$\begin{aligned}
&\left|\zeta(tn^{-1/2})^n - \xi(t)\right| \\
&\leq \exp\left(-\frac{1}{2}\|t\|_2^2\right) \max\left\{\exp|u(t)|, \exp|v(t)|\right\} \left(|u(t) - v(t)| + \frac{|v(t)|^{k-1}}{(k-1)!}\right) \\
&\leq \exp\left(-\frac{1}{2}\|t\|_2^2\right) \max\left\{\exp\left(\frac{1}{4}\|t\|_2^2\right), \exp\left(C\|t\|_2^3 n^{-1/2}\right)\right\} \\
&\cdot \left(\frac{\epsilon\|t\|_2^k}{n^{k/2-1}} + \frac{C_p^{k-1}\|t\|_2^{3(k-1)}}{n^{k/2-1/2}k!}\right) \\
&\leq \exp\left(-\frac{1}{4}\|t\|_2^2\right) \left[\frac{\epsilon\|t\|_2^k}{n^{k/2-1}} + \frac{C_p^{k-1}\|t\|_2^{3(k-1)}}{(k-1)!n^{k/2-1/2}}\right].
\end{aligned}$$

□

Note that this proof doesn't use the fact that ζ is a characteristic function. Indeed, this theorem can be proven in a more general setting without any changes to the statement of the theorem or the proof itself.

We finally prove the main theorem of this section by relating the error of the Edgeworth approximation to the error of the associated Fourier transforms. The original proof is presented in [20, Theorem 3.5.1].

Theorem 2.12. Let P be a distribution and $k \in \mathbb{N}_{\geq 2}$ such that all cumulants $\kappa(X)$ of P of order up to k exist. Let $n \in \mathbb{N}$, let $X_1, \ldots, X_n \overset{iid}{\sim} P$ and Y be the standardized sum

$$Y = n^{-1/2} \sum_{i=1}^{n} X_i.$$

Let $e_{k,n}(\cdot; \kappa(X))$ be the Edgeworth series, constructed by only keeping cumulants of order up to k in (2.8). Then, if the density f_Y of Y exists, $e_{k,n}(\cdot; \kappa(X))$ approximates f_Y with a uniform error of order $o(n^{1-k/2})$.

Proof. Without loss of generality, we assume that, for $i \in [n]$, X_i has mean 0 and a covariance matrix equal to the identity, see Remark 2.8. Let ξ be the Fourier transform of $e_{k,n}(\cdot;\kappa(X))$, then by Corollary 2.2, we can bound, for any $y \in \mathbb{R}^p$, the absolute difference between $f_Y(y)$ and $e_{k,n}(y;\kappa(X))$ by

$$|f_Y(y) - e_{k,n}(y;\kappa(X))| \leq (2\pi)^{-p} \int_{\mathbb{R}^p} |\zeta(tn^{-1/2})^n - \xi(t)| \mathrm{d}t, \tag{2.16}$$

where $\zeta(tn^{-1/2})^n$ is the characteristic function of Y. Since both ζ and ξ are $L^1(\mathbb{R}^p)$, the integral is well defined and provides a valid upper bound. We proceed by splitting the range of integration in two parts: one part in which t is small such that Theorem 2.11 can be applied, and the remaining part of the integral will be handled separately.

By construction of the Edgeworth approximation, the Fourier transform of $e_{k,n}(\cdot;\kappa(X))$ corresponds to the function given in (2.14) of Theorem 2.11. Hence, for any $\varepsilon > 0$, there exists $\delta > 0$ such that (2.15) holds and we can upper bound the *small* t part of the right hand side of (2.16) as follows,

$$\begin{aligned}
&\int_{B_2(\delta\sqrt{n})} |\zeta(tn^{-1/2})^n - \xi(t)| \mathrm{d}t \\
&\qquad \leq (2\pi)^{-p} \int_{B_2(\delta\sqrt{n})} \exp\left(-\frac{1}{4}\|t\|_2^2\right) \left[\frac{\epsilon \|t\|_2^k}{n^{k/2-1}} + \frac{C_0^{k-1}\|t\|_2^{3(k-1)}}{(k-1)!n^{k/2-1/2}}\right] \mathrm{d}t \\
&\qquad \leq \frac{\epsilon C_1}{n^{(k-2)/2}} \mathbb{E}_T\left[\|T\|_2^k\right] + \frac{C_2^k}{k!n^{(k-1)/2}} \mathbb{E}_T\left[\|T\|_2^{3k}\right] = o(n^{1-k/2}),
\end{aligned}$$

in which $T \sim N(0, 2\mathbb{1}_p)$ and $C_0, C_1, C_2 \in \mathbb{R}$ are constants that do not depend on n.

For the remaining part of the integral, where $\|t\|_2 \geq \delta\sqrt{n}$, we bound the integral by the triangle inequality and consider each term separately,

$$\begin{aligned}
&\int_{\mathbb{R}^p \setminus B_2(\delta\sqrt{n})} |\zeta(tn^{-1/2})^n - \xi(t)| \mathrm{d}t \\
&\qquad \leq \int_{\mathbb{R}^p \setminus B_2(\delta\sqrt{n})} |\xi(t)| \mathrm{d}t + \int_{\mathbb{R}^p \setminus B_2(\delta\sqrt{n})} |\zeta(tn^{-1/2})^n| \mathrm{d}t \\
&\qquad = I_1 + I_2.
\end{aligned}$$

By construction of ξ, the integral I_1 has an exponential decay, thus I_1 is $o(n^{1-k/2})$. As for the integral I_2, using that $|\zeta(t)| < 1$ for $t \neq 0$ and $|\zeta(t)| \to 0$ for $n \to \infty$ and any $t \in \mathbb{R}^p$, there exists $a \in (0,1)$ such that for n large enough, if $\|t\|_2 \geq \delta\sqrt{n}$, then $|\zeta(tn^{-1/2})| \leq a$. Furthermore, by assumption of the existence of f_Y and Lemma 2.3, there exists $q > 1$

such that $\zeta^n \in L^q(\mathbb{R}^p)$. Thus,

$$I_2 \leq a^{n-q} \int_{\mathbb{R}^p \setminus B_2(\delta\sqrt{n})} |\zeta(tn^{-1/2})|^q \mathrm{d}t \leq a^{n-q}\sqrt{n} \int_{\mathbb{R}^p} |\zeta(t)|^q \mathrm{d}t = O(\sqrt{n}a^n) = o(n^{1-k/2}),$$

which concludes the proof. □

2.4 A numerical case study of the Edgeworth approximation

To better understand the Edgeworth approximation, we investigate its behaviour when applied to a distribution for which the true density of the standardized sum is known. This is the case for the Gamma distribution as presented in [20, Section 3.6].

Example 2.13. The Gamma distribution $\Gamma(p, \lambda)$ for $p, \lambda > 0$ has density

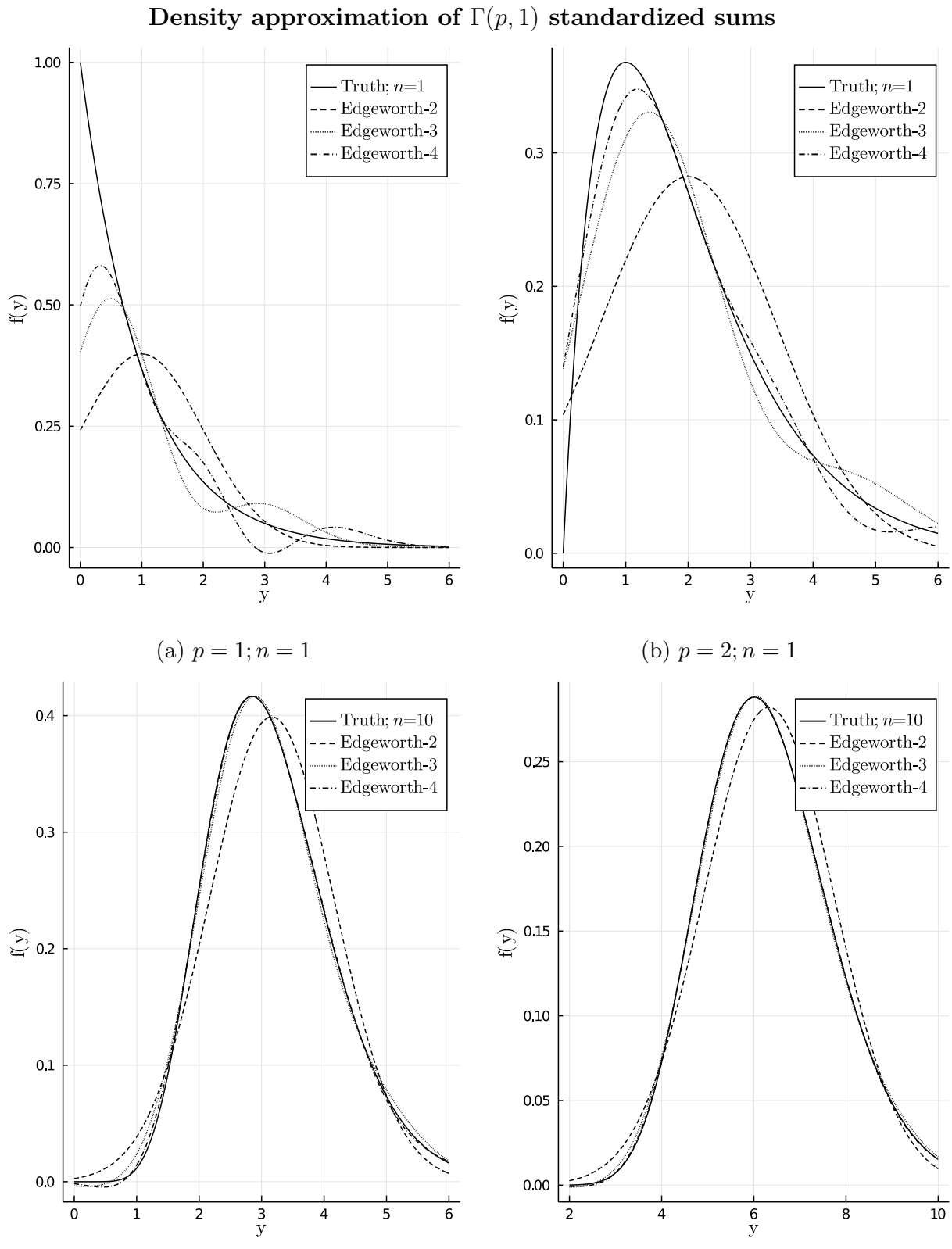
$$f(x) = \frac{\lambda^p}{\Gamma(p)} x^{p-1} \exp(-\lambda x),$$

where Γ is the Gamma function. Its characteristic function is $\zeta(t) = (1 - it/\lambda)^{-p}$. Hence, we can easily see that for $X_1, \ldots, X_n \overset{iid}{\sim} \Gamma(p, \lambda)$, both the sum and standardized mean of $X_1, \ldots, X_n$ follow a Gamma distribution with $\sum_{i=1}^n X_i \sim \Gamma(np, \lambda)$ and $n^{-1/2}\sum_{i=1}^n X_i \sim \Gamma(np, \lambda n^{-1/2})$. The cumulant generating function of the $\Gamma(p, \lambda)$ distribution is

$$K(t) = p\log(\lambda) - p\log(\lambda - t),$$

hence the (j)-cumulant of X is $\kappa_{(j)} = p\Gamma(j)\lambda^{-j}$. To be able to apply Theorem 2.12, the density of the standardized sum must exist, which is true since we know that it follows a Gamma distribution.

In Figure 1, we show several examples of the behaviour of the Edgeworth approximation under different conditions. In the upper pane of Figure 1, we compare the Edgeworth approximations of orders $k = 2, 3, 4$ to the true density of a standardized sum of $n = 1$ and $n = 10$ random variables with a $\Gamma(p, 1)$ distribution for $p = 1, 2$. For $p = 1$, $\Gamma(p, 1)$ is an exponential distribution. For $n = 1$, the discontinuity at $y = 0$ of the exponential distribution results in high oscillations of the Edgeworth approximation as demonstrated in Figure 1a which even leads to negative values of the density approximation. Increasing to $p = 2$, we can see in Figure 1b that the approximation is better behaved but unsurprisingly still does not well approximate the $\Gamma(2, 1)$ distribution. For both $p = 1$ and $p = 2$, increasing the number of terms summed to $n = 10$ results in seemingly good approximations to the density of the standardized sum as shown in Figures 1c and 1d.



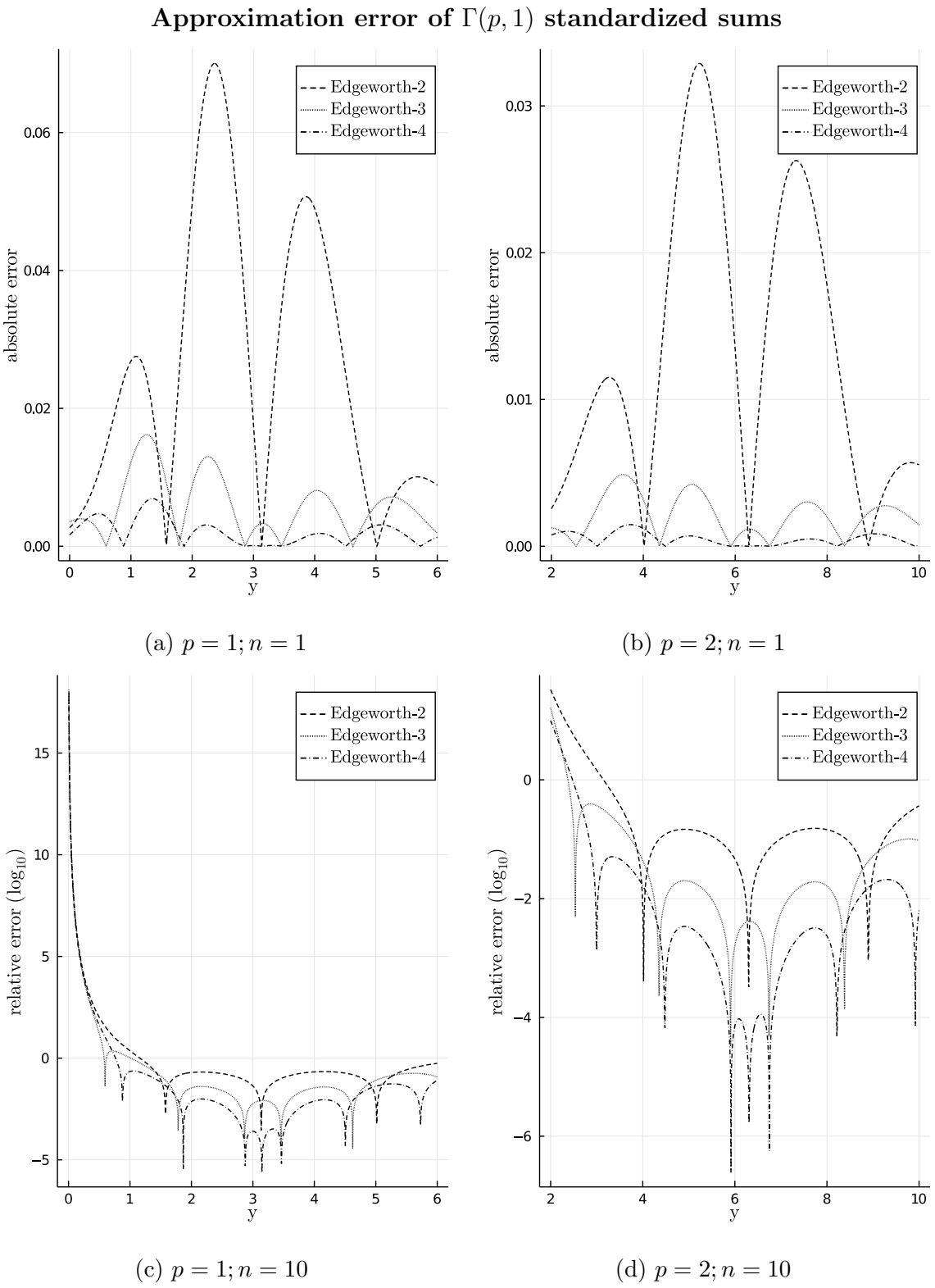
(a) $p = 1; n = 1$

(b) $p = 2; n = 1$

(c) $p = 1; n = 10$

(d) $p = 2; n = 10$

Figure 1: Several combinations of p and n exposing different behaviours of the Edgeworth approximation to the density of a standardized sum of n i.i.d. random variables following a $\Gamma(p, 1)$ distribution.



(a) $p = 1; n = 1$

(b) $p = 2; n = 1$

(c) $p = 1; n = 10$

(d) $p = 2; n = 10$

Figure 2: Study of the approximation error of the Edgeworth approximation on a standardized sum of $n = 10$ i.i.d. random variables following a $\Gamma(p, 1)$ distribution. The absolute error studied in Theorem 2.12 is well behaved as shown in the upper pane. However, the lower pane shows that the relative error of the approximation can be extremely high in low density regions where a low absolute error might still be a large relative error.

While Figure 1 appears to show good results of the Edgeworth approximation, it is hard to assess the quality of the approximations in regions of low probability. We display in Figure 2 the error of the Edgeworth series of orders $k = 2, 3, 4$ approximating the density of a standardized sum of $n = 10$ i.i.d. random variables following a $\Gamma(p, 1)$ distribution for $p = 1$ and $p = 2$. The upper pane demonstrates the control of the absolute approximation error studied in Theorem 2.12. However, the lower pane of Figure 2 shows that the relative error can still reach very high values even as the order of the approximation increases. This is explained by the fact that even if the relative error is controlled, it might still be big relative to the true density in low probability regions.

In many settings, one is interested in using distribution approximations to compute p-values in statistical tests. In this case, one is trying to find statistical evidence against a null hypotheses by demonstrating a low p-value of the null hypothesis model. Hence, the Edgeworth series itself can be ill suited for direct applications. However, as we will see in the next section, the Edgeworth approximation and related approximation results can still be used to construct approximations that are usable to estimate the density function in low probability regions.

2.5 Saddlepoint approximation

This section presents another approximation scheme based on the Edgeworth approximation, which resolves some of the issues of the Edgeworth approximation highlighted in the previous section.

We begin by introducing *exponential tilting*. Consider a random variable $X \in \mathbb{R}^p$ with cumulant generating function K and density f. We introduce the exponential family $\mathcal{T}_P = \{P_\gamma\}_{\gamma \in \mathbb{R}^p}$ where each $P_\gamma \in \mathcal{T}_P$ is characterized by its density function $f(\cdot; \gamma)$ given by

$$f(x; \gamma) = f(x) \exp\left(\gamma^\top x - K(\gamma)\right).$$

Note that by the definition of the cumulant generating function, $K(\gamma)$ is the correct normalization factor for $f(\cdot; \gamma)$ to integrate to 1, and hence $f(\cdot; \gamma)$ is a valid density function. Furthermore, the original distribution P is an element of $\mathcal{T}_P$ with $P = P_0$. Given two distributions $P_{\gamma_0}, P_\gamma \in \mathcal{T}_P$, their densities differ by a known factor

$$f(x; \gamma_0) = f(x; \gamma) \exp\left((\gamma_0 - \gamma)^\top x - [K(\gamma_0) - K(\gamma)]\right).$$

Hence, choosing $\gamma_0 = 0$ gives $f(\cdot; \gamma_0) = f$ and the following holds for any $\gamma \in \mathbb{R}^p$,

$$f(x) = f(x; \gamma) \exp\left(K(\gamma) - \gamma^\top x\right). \tag{2.17}$$

Therefore, we can construct an approximation of f by choosing γ such that $f(\cdot;\gamma)$ can be accurately approximated.

Let us now consider a distribution P with cumulant generating function K. We wish to use the previous argumentation to approximate the density f_n of the mean S of n i.i.d. random variables distributed according to P. Using that the cumulant generating function of S is $K_n(t) = nK(t/n)$ and replacing it in (2.17), we get

$$f_n(s) = f_n(s;\gamma)\exp\left(nK(\gamma/n) - \gamma^\top s\right), \tag{2.18}$$

where $f_n(\cdot;\gamma)$ is the density of the mean of n i.i.d. random variables distributed according to P_γ. Since the Edgeworth approximation was derived for a standardized sum of random variables, we apply the transformation

$$\begin{aligned}\frac{1}{n}\sum_{i=1}^{n} X_i &\mapsto \frac{1}{\sqrt{n}}\sum_{i=1}^{n}\Sigma_\gamma^{-1/2}(X_i - \mu_\gamma)\\ s &\mapsto s^* := \sqrt{n}\Sigma_\gamma^{-1/2}(s-\mu_\gamma)\end{aligned}$$

where μ_γ and Σ_γ are respectively the mean and covariance under the distribution P_γ. Furthermore, the determinant of the transformation is $n^{p/2}|\Sigma_\gamma|^{-1/2}$, which gives, using the notation in (2.11),

$$f_n(s;\gamma) = n^{p/2}|\Sigma_\gamma|^{-1/2}\phi(s^*)\left\{1 + P_{k,n}(s^*;\kappa(\gamma)) + o(n^{1-k/2})\right\}, \tag{2.19}$$

where $\kappa(\gamma)$ are the cumulants of the random variable distributed according to P_γ. The cumulant generating function $K(\cdot;\gamma)$ of P_γ can be expressed in terms of the cumulant generating function K by

$$K(t;\gamma) = K(t+\gamma) - K(\gamma).$$

Since the covariance matrix Σ_γ is equal to the Hessian of the cumulant generating function $K(\cdot;\gamma)$ of P_γ evaluated at 0, we have $\Sigma_\gamma = K''(\gamma)$. This lets us rewrite (2.19) in terms of K as follows,

$$f_n(s;\gamma) = n^{p/2}|K''(\gamma)|^{-1/2}\phi(s^*)\left\{1 + P_{k,n}(s^*;\kappa(\gamma)) + o(n^{1-k/2})\right\}.$$

We are now interested in choosing γ such that the Edgeworth approximation of $f_n(\cdot;\gamma)$ is accurate. As seen in Remark 2.9, the Edgeworth approximations of even order k have an approximation error of $O(n^{-k/2})$ instead of $o(n^{1-k/2})$ when evaluated at the mean of the distribution. In other words, the Edgeworth approximation will be more accurate if

$s^* = 0$ in the previous equation. Since γ can be chosen freely and differently for each value s at which the density f_n is evaluated, we can choose γ such that $s^* = 0$, or equivalently, such that $s = \mu_\gamma$. Similarly to the covariance matrix, we can write the mean of P_γ as $\mu_\gamma = K'(\gamma)$. Hence, for any $s \in \mathbb{R}^p$, we find a distribution $P_{\hat{\gamma}_s} \in \mathcal{T}_P$ with mean s by solving

$$K'(\hat{\gamma}_s) = s. \tag{2.20}$$

We call the solution of this equation $\hat{\gamma}_s$ to emphasize the fact that for each $s \in \mathbb{R}^p$, a different tilting distribution $P_{\hat{\gamma}_s}$ is chosen such that the Edgeworth approximation to the density of $P_{\hat{\gamma}_s}$ is accurate in s. Note that if $\hat{\gamma}_s$ solves (2.20), it is also the maximum likelihood estimator of γ within the model $\mathcal{T}_P$. Replacing γ by $\hat{\gamma}_s$ in (2.19), we get

$$f_n(s; \hat{\gamma}_s) = \left(\frac{n}{2\pi}\right)^{p/2} |\Sigma_{\hat{\gamma}_s}|^{-1/2} \left\{1 + P_{k,n}(0; \kappa(\hat{\gamma}_s)) + O(n^{-k/2})\right\}.$$

Replacing $f_n(s; \gamma)$ by the approximation above in (2.18) gives

$$\begin{aligned} f_n(s) &= \left(\frac{n}{2\pi}\right)^{p/2} \frac{\exp\left(nK(\hat{\gamma}_s/n) - \hat{\gamma}_s^\top s\right)}{|K''(\hat{\gamma}_s)|^{1/2}} \left[1 + P_{k,n}(0; \kappa(\hat{\gamma}_s)) + O(n^{-k/2})\right] \\ &= g(s; K) \left[1 + P_{k,n}(0; \kappa(\hat{\gamma}_s)) + O(n^{-k/2})\right] \end{aligned} \tag{2.21}$$

where

$$g(s; K) = \left(\frac{n}{2\pi}\right)^{p/2} \frac{\exp\left(nK(\hat{\gamma}_s/n) - \hat{\gamma}_s^\top s\right)}{|K''(\hat{\gamma}_s)|^{1/2}}.$$

We call $g(\cdot; K)$ the *Saddlepoint approximation* to the density of S. We now justify the approximation accuracy claim from (2.21) in the following theorem.

Theorem 2.14. Let P be a distribution with cumulant generating function K and $k \in \mathbb{N}_{>2}$ such that all cumulants of P of order up to k exist. Suppose that for every $s \in \mathbb{R}^p$, (2.20) has a unique solution $\hat{\gamma}_s$. Let $n \in \mathbb{N}$ and S be the mean of $X_1, \ldots, X_n \overset{iid}{\sim} P$,

$$S = n^{-1} \sum_{i=1}^{n} X_i.$$

Then, if the density f_n of S exists, the expansion given in (2.21) holds.

Proof. This result is a direct consequence of Theorem 2.12, applied pointwise to the tilted distribution $P_{\hat{\gamma}_s}$ for every $s \in \mathbb{R}^p$. As discussed above, Remark 2.9 implies that only powers of n^{-1} have non-vanishing coefficients in the Edgeworth approximation of the tilted densities. This turn implies that the Edgeworth approximation error in each point

is of order $O(n^{-k/2})$, concluding the proof of the theorem. □

While the Saddlepoint approximation has many advantages over the Edgeworth approximation, it is important to note that the Saddlepoint approximation requires the complete cumulant generating function of the approximated density to be known. The Edgeworth approximation on the other hand only uses the first k cumulants of the distributions, which are evaluations of derivatives of the cumulant generating function in 0.

A special case of particular interest arises when taking $k = 2$. In this case, the Edgeworth approximation of $f_n(\cdot; \hat{\gamma}_s)$ is equal to its normal approximation since the polynomial part $P_{k,n}(\cdot; \kappa(\hat{\gamma}_s))$ of $e_{k,n}(\cdot; \kappa(\hat{\gamma}_s))$ is equal to 0, giving

$$\begin{aligned} f_n(s) &= g(s; K)\left[1 + O(n^{-1})\right] \\ &= \left(\frac{n}{2\pi}\right)^{p/2} \frac{\exp\left(nK(\hat{\gamma}_s/n) - \hat{\gamma}_s^\top s\right)}{|K''(\hat{\gamma}_s)|^{1/2}} \left[1 + O(n^{-1}))\right]. \end{aligned} \tag{2.22}$$

The Saddlepoint approximation of second order is commonly used in applications since it presents many advantages compared to the Edgeworth approximation. It has a simple expression which makes it easier to construct and manipulate it. Furthermore, the Saddlepoint approximation is often highly accurate or even exact up to normalization, and, unlike the other approximations presented so far, it is always positive.

Example 2.15. Extending Example 2.13, we analyze the behaviour of the Saddlepoint approximation to the mean $Y = n^{-1}\sum_{i=1}^n X_i \in \mathbb{R}_+$ where $X_1, \ldots, X_n \overset{iid}{\sim} \Gamma(p, \lambda)$. The cumulant generating function of the $\Gamma(n, p)$ distribution is $K(t) = p\log(\lambda) - p\log(\lambda - t)$ and its first derivative is $K'(t) = p/(\lambda - t)$. For any $s \in \mathbb{R}_+$, the Saddlepoint $\hat{\gamma}_s$ is given by the solution to the Saddlepoint Equation in (2.20), which here becomes

$$\frac{p}{\lambda - \hat{\gamma}_s/n} = s \Rightarrow \hat{\gamma}_s = n\left(\lambda - \frac{p}{s}\right).$$

In Figure 3, we demonstrate how the Saddlepoint approximation of second order compares to the Edgeworth approximation when approximating a standardized sum of n random variables independently distributed according to $\Gamma(2, 1)$. Since the standardized sum can be obtained by multiplying the mean by a factor of $\sqrt{n}$, the Saddlepoint approximation is easily adapted by change of variable. Both panes show accurate approximation properties both in terms of relative and absolute error.
In this example, it is also interesting to examine the explicit form of the Saddlepoint approximation g. Replacing the relevant quantities in (2.22), we obtain that the Saddlepoint

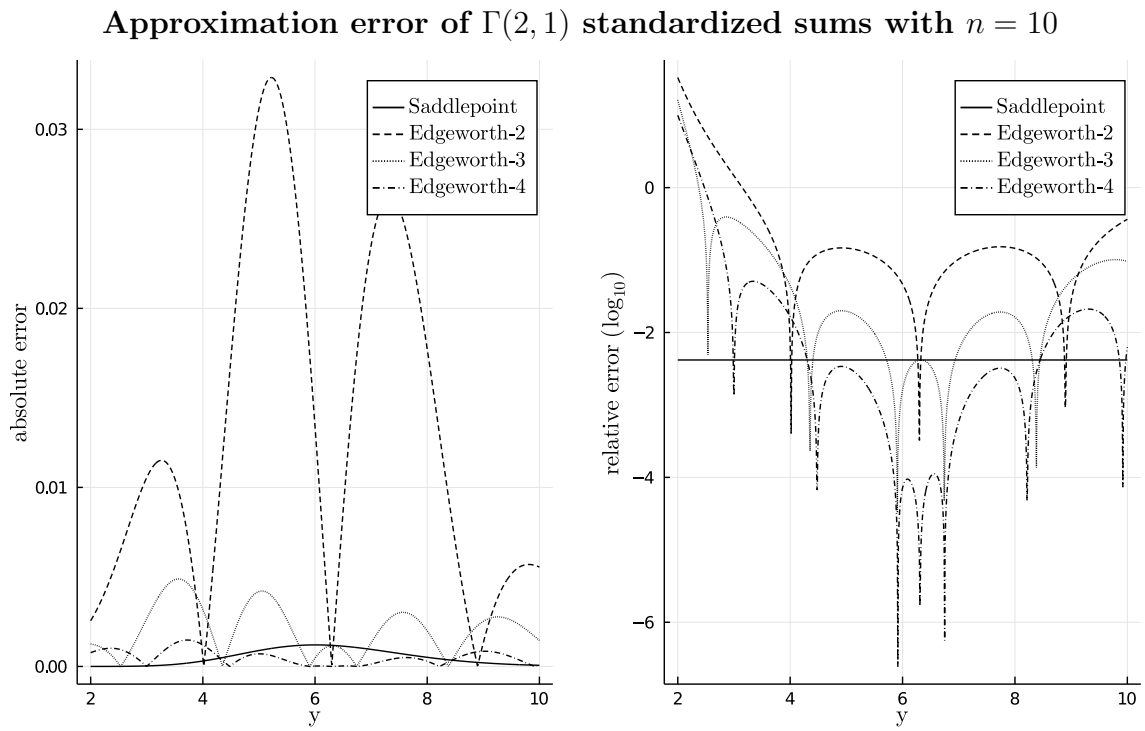


Figure 3: Study of the error of the Saddlepoint approximation on a standardized sum $n = 10$ i.i.d. random variables distributed according to $\Gamma(2, 1)$. Both panes demonstrate the properties studied of the Saddlepoint approximation: the accurate relative error, the gain in order of approximation and the uniform relative error of the approximation for sums of Gamma random variables.

approximation is

$$\begin{aligned} g(s;K) &= \sqrt{\frac{n}{2\pi K''(\lambda - \frac{p}{s})}} \exp\left(nK\left(\lambda - \frac{p}{s}\right) - n\left(\lambda - \frac{p}{s}\right)s\right) \\ &= \sqrt{\frac{n}{2\pi s^2/p}} \exp\left(n\left(p\log\left(\lambda\right) - p\log\left(p/s\right)\right) - ns\lambda + np\right) \\ &= (n\lambda)^{np} s^{np-1} \exp\left(-sn\lambda\right) \frac{(np)^{1/2-np}\exp\left(np\right)}{\sqrt{2\pi}}. \end{aligned}$$

Consider now Stirling's formula for the gamma function

$$\Gamma(z) \approx \sqrt{2\pi} z^{z-1/2} \exp\left(-z\right).$$

We recognize that the second term in the expression of $g(s;K)$ corresponds to the inverse of Stirling's approximation of $\Gamma(np)$. Therefore, the Saddlepoint approximation to the density of the mean of n i.i.d. random variables distributed according to $\Gamma(p,\lambda)$ corresponds to the density of the true distribution $\Gamma(np, n\lambda)$ of the mean, where the gamma function has been replaced by Stirling's approximation. This has the consequence that the relative error of the Saddlepoint approximation does not depend on s, the point at which the density is evaluated, but rather only depends on n. This behaviour is also seen in Figure 3 where the relative error of the Saddlepoint approximation is a straight horizontal line. Daniels [13] characterizes the class of distributions for which the uniform relative approximation error holds.

2.6 The p^* approximation in exponential families

Next, we apply the Saddlepoint approximation to an exponential family $\mathcal{P} = \{P_\theta\}_\theta$ with natural parameter $\theta \in \mathbb{R}^p$. We write $f(\cdot;\theta)$ for the density of $P_\theta \in \mathcal{P}$. Then, $f(\cdot;\theta)$ is given by

$$f(x;\theta) = \exp\left(\theta^\top T(x) - \mathcal{H}(\theta) - \mathcal{G}(x)\right).$$

Given a random sample $x = (x_1, \ldots, x_n)$ of P_θ, the *log-likelihood function* denoted by $\ell(\cdot;x)$ is given by

$$\ell(\theta;x) = \theta^\top \sum_{i=1}^{n} T(x_i) - n\mathcal{H}(\theta) = n\left[\bar{t} - \mathcal{H}(\theta)\right],$$

where $\bar{t} = n^{-1}\sum_{i=1}^{n} T(x_i)$ is the sample average of the sufficient statistic T. Hence, the maximum likelihood estimator of θ is the value $\hat{\theta}_{\bar{t}} \in \mathbb{R}^p$ satisfying the score equation

$$\mathcal{H}'(\hat{\theta}_{\bar{t}}) = \bar{t}. \tag{2.23}$$

For simplicity, we assume that $\mathcal{H}'$ is one-to-one to ensure that (2.23) has a unique solution $\hat{\theta}_{\bar{t}}$. In the exponential family $\mathcal{P}$, it can be shown that the cumulant generating function of any member $P_\theta \in \mathcal{P}$ is given by $K_\theta(t) = \mathcal{H}(\theta + t) - \mathcal{H}(\theta)$. Thus $K'_\theta(t) = \mathcal{H}'(\theta + t)$. Using the cumulant generating function in the score equation (2.23) gives

$$K'_\theta(\hat{\theta}_{\bar{t}} - \theta) = \bar{t}.$$

Consider the Saddlepoint equation given in (2.20), and notice that the parameter $\hat{\gamma}_{\bar{t}}$ of the tilted family is related to the maximum likelihood estimator $\hat{\theta}$ by

$$\hat{\gamma}_{\bar{t}}/n = \hat{\theta}_{\bar{t}} - \theta.$$

Using this in the Saddlepoint approximation (2.22), we obtain that the Saddlepoint approximation for the average $\bar{T} = n^{-1}\sum_{i=1}^{n} T(X_i)$, where $X_1, \ldots, X_n \overset{iid}{\sim} P_\theta$, is

$$\begin{aligned} g(\bar{t}; K_\theta) &= \left(\frac{n}{2\pi}\right)^{p/2} |K''_\theta(\hat{\theta}_{\bar{t}} - \theta)|^{-1/2} \exp\left(nK_\theta(\hat{\theta}_{\bar{t}} - \theta) - (\hat{\theta}_{\bar{t}} - \theta)^\top \bar{t}\right) \\ &= \left(\frac{n}{2\pi}\right)^{p/2} |\mathcal{H}''(\hat{\theta}_{\bar{t}})|^{-1/2} \exp\left(n(\mathcal{H}(\hat{\theta}_{\bar{t}}) - \mathcal{H}(\theta)) - (\hat{\theta}_{\bar{t}} - \theta)^\top \bar{t}\right) \\ &= \left(\frac{n}{2\pi}\right)^{p/2} |j(\hat{\theta}_{\bar{t}})|^{-1/2} \exp\left(\ell(\theta; \bar{t}) - \ell(\hat{\theta}_{\bar{t}}; \bar{t})\right), \end{aligned}$$

where the last equality follows from the fact that $\mathcal{H}''(\hat{\theta})$ is equal to the observed Fisher information $j(\hat{\theta})$. Daniels [1] notes that this approximation can further be used to approximate the distribution of the maximum likelihood estimator. Let $\hat{\Theta}$ be the random variable solving the score equation $\mathcal{H}'(\hat{\Theta}) = \bar{T}$. By change of variable, we can use the approximation above to construct the p^* *approximation* to the density of $\hat{\Theta}$, given by

$$p^*(\hat{\theta}; \theta, \bar{t}) = \left(\frac{n}{2\pi}\right)^{p/2} |j(\hat{\theta})|^{-1/2} \exp\left(\ell(\theta; \bar{t}) - \ell(\hat{\theta}; \bar{t})\right) \left|\frac{\mathrm{d}\hat{\theta}}{\mathrm{d}\bar{t}}\right|^{-1}.$$

To compute the determinant of the Jacobian of the transformation $\hat{\theta}(\bar{t})$, we differentiate the score equation with respect to $\hat{\theta}$ to find $\mathcal{H}''(\hat{\theta}) = (\mathrm{d}\bar{t}/\mathrm{d}\hat{\theta})$ and hence $(\mathrm{d}\hat{\theta}/\mathrm{d}\bar{t}) = \mathcal{H}''(\hat{\theta})^{-1} = j(\hat{\theta})^{-1}$. Therefore, the density of $\hat{\Theta}$ given the true parameter θ and the obser-

vation $\bar{t}$ is approximated by

$$p^*(\hat{\theta};\theta,\bar{t}) = \left(\frac{n}{2\pi}\right)^{p/2} |j(\hat{\theta})|^{1/2} \exp\left(\ell(\theta;\bar{t}) - \ell(\hat{\theta};\bar{t})\right). \tag{2.24}$$

While the dependence on $\bar{t}$ naturally comes from the proposed derivation of the p^* approximation, it is often more convenient to parametrize the loglikelihood $\ell(\cdot;x)$ and p^* approximations in terms of the maximum likelihood estimator $\hat{\theta}(\bar{t})$. We then write

$$p^*(\hat{\theta};\theta,\hat{\theta}) = \left(\frac{n}{2\pi}\right)^{p/2} |j(\hat{\theta})|^{1/2} \exp\left(\ell(\theta;\hat{\theta}) - \ell(\hat{\theta};\hat{\theta})\right).$$

This highlights the fact that the p^* approximation inherits its locality from the Saddlepoint approximation, since the density $p^*(\hat{\theta};\theta,\hat{\theta})$ is different at each point $\hat{\theta}$ at which it is evaluated. The p^* approximation can also be used in many different situations where the distribution of refence is not necessarily an exponential family. Several articles and books by Barndorff-Nielsen[2, 3] and other authors study and derive the p^* approximation in broader generality.

Suppose now that the exponential family $\mathcal{P}$ has an alternative parametrization $\{P_\phi\}$ such that there exists a diffeomorphism $\phi = \phi(\theta)$ satisfying $\hat{\phi} = \phi(\hat{\theta})$, where $\hat{\phi}$ and $\hat{\theta}$ are the maximum likelihood estimators in their respective parametrizations. Then,

$$\begin{aligned}
p^*(\hat{\phi};\phi,\hat{\phi}) &= \left(\frac{n}{2\pi}\right)^{-p/2} |j_\phi(\hat{\phi})|^{1/2} \exp\left(\ell(\phi;\hat{\phi}) - \ell(\hat{\phi};\hat{\phi})\right) \\
&= \left(\frac{n}{2\pi}\right)^{-p/2} \left(|j_\theta(\theta(\hat{\phi}))| \left|\frac{\mathrm{d}\hat{\theta}}{\mathrm{d}\hat{\phi}}\right|^{-2}\right)^{1/2} \exp\left(\ell(\theta(\phi);\theta(\hat{\phi})) - \ell(\theta(\hat{\phi});\theta(\hat{\phi}))\right) \\
&= p^*(\theta(\hat{\phi});\theta(\phi),\theta(\hat{\phi})) \left|\frac{\mathrm{d}\hat{\theta}}{\mathrm{d}\hat{\phi}}\right|^{-1}.
\end{aligned}$$

Hence, the p^* approximation is invariant under reparametrization. The next example demonstrates the use of the p^* approximation and shows how the parameterization invariance can be useful when applying the approximation.

Example 2.16. We estimate the density of the maximum likelihood estimator of the parameter $\lambda \in \mathbb{R}_+$ of an exponential distribution $\mathrm{Exp}(\lambda)$. The density of the distribution $\mathrm{Exp}(\lambda)$ is

$$f_\lambda(x) = \lambda \exp(-\lambda x).$$

To make direct use of the p^* approximation in (2.24), we must work in the natural parametrization of the exponential distribution. For $\lambda \in R_+$, the corresponding natural

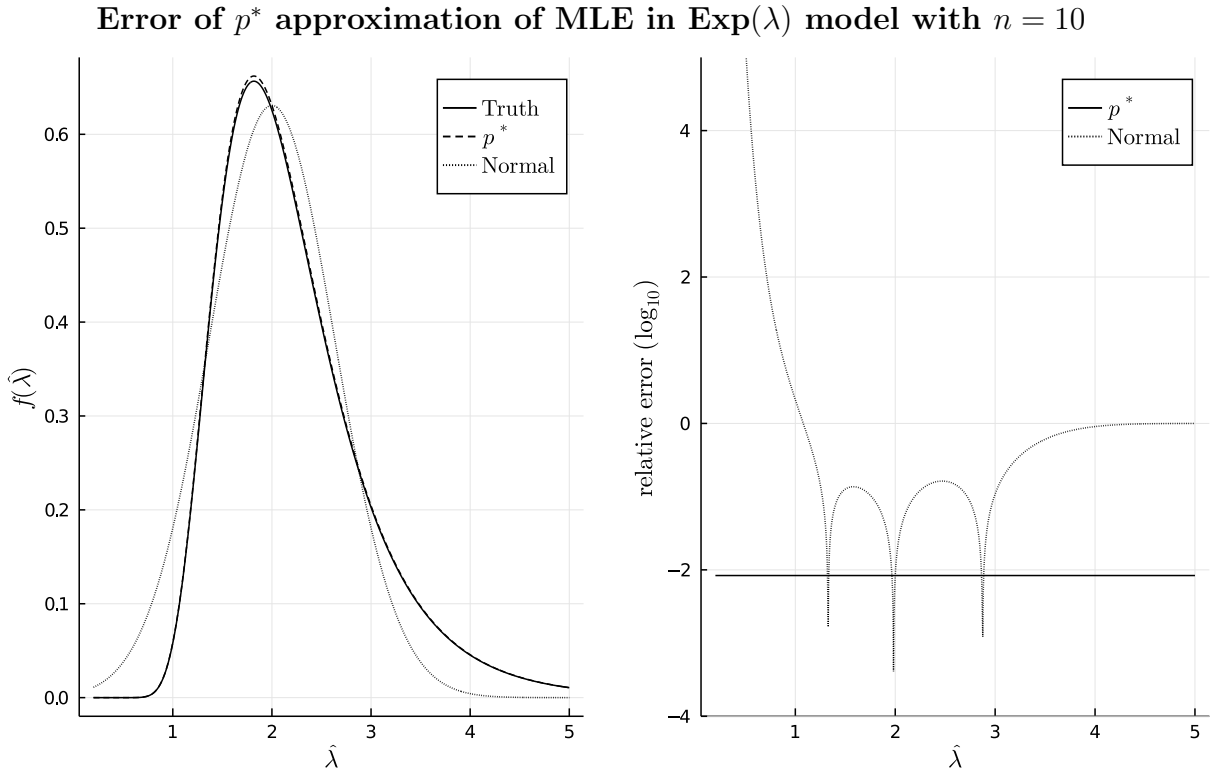


Figure 4: Study of the approximation error of the Saddlepoint approximation on a standardized sum of $n = 10$ of $\Gamma(2, 1)$ random variables. Both panes expose properties studied of the Saddlepoint approximation: the accurate relative error, the gain in order of approximation and the uniform relative error of the approximation for sums of Gamma random variables.

parameter is $\theta = -\lambda \in \mathbb{R}_-$ and the density of $\text{Exp}(\theta)$ is then $f_\theta(x) = \exp(\theta x + \log(-\theta))$. Given an i.i.d. sample $x_1, \ldots, x_n$ of $\text{Exp}(\theta)$, the log-likelihood function is given by

$$\ell(\theta; \bar{x}) = n\left[\theta\bar{x} + \log(-\theta)\right],$$

where we used that the sufficient statistic is $T(x) = x$ and hence $\bar{t} = \bar{x}$ is the sample mean. The maximum likelihood estimator of θ is then $\hat{\theta} = -1/\bar{x}$ and the observed information is equal to $j(\theta) = 1/\theta^2$.
It follows that the p^* approximation to the density of $\hat{\theta}$ is

$$\begin{aligned} p^*(\hat{\theta}; \theta, \hat{\theta}) &= \sqrt{n}\frac{|\theta|^n}{|\hat{\theta}|^{n-1}} \exp\left(-n(\theta - \hat{\theta})/\hat{\theta}\right)/\sqrt{2\pi} \\ &= \sqrt{n}\frac{|\theta|^n}{|\hat{\theta}|^{n-1}} \exp\left(n\left[1 - \frac{\theta}{\hat{\theta}}\right]\right)/\sqrt{2\pi}. \end{aligned}$$

Using the invariance of the p^* approximation, we obtain a p^* approximation of the density of the maximum likelihood parameter $\hat{\lambda}$ in the original parametrization,

$$\begin{aligned} p^*(\hat{\lambda}; \lambda, \hat{\lambda}) &= p^*(\theta(\hat{\lambda}); \theta(\lambda), \theta(\hat{\lambda}))\left|\mathrm{d}\hat{\theta}/\mathrm{d}\hat{\lambda}\right|^{-1} \\ &= \sqrt{n}\frac{|\lambda|^n}{|\hat{\lambda}|^{n-1}} \exp\left(n\left[\frac{\lambda}{\hat{\lambda}} - 1\right]\right)/\sqrt{2\pi}. \end{aligned} \tag{2.25}$$

The Normal approximation is a commonly used approximation to the distribution of the maximum likelihood estimator. In the exponential model, the Fisher information is $I(\lambda) = \lambda^{-2}$ and the following central limit theorem holds for the maximum likelihood estimator [22, Example 3.12]

$$\sqrt{n}(\hat{\lambda} - \lambda) \xrightarrow{\mathrm{d}} N(0, I(\lambda)^{-1}) \quad \text{as } n \to \infty. \tag{2.26}$$

Hence, $\hat{\lambda}$ is approximately $N(\lambda, \lambda^2/n)$ with an approximation error of the density of $o(n^{-1/2})$.

In Figure 4, we display how (2.25) and (2.26) approximate the density of $\hat{\lambda}$ under the true model $\text{Exp}(2)$. Since $\text{Exp}(\lambda) = \Gamma(1, \lambda)$, the distribution of $\bar{X}$ is $\Gamma(n, n\lambda)$ and hence $\hat{\lambda} = \bar{x}$ is Inv-$\Gamma(n, n\lambda)$. As we can see in the left pane, the p^* approximation properly fits the true density of $\hat{\lambda}$ and captures the bias of the $\hat{\lambda}$ estimator as opposed to the Normal approximation which is centered around the true value of λ. Furthermore, we observe in the right panel how the relative error of the p^* approximation is identical to the approximation error of the Saddlepoint approximation to the mean of $\Gamma(2, 1)$ seen in

Example 2.15. This is also a direct consequence of the invariance of the p^* approximation since $\hat{\Lambda}$, the random variable associated to the maximum likelihood estimator, is the inverse of the sample mean $\bar{X}$, which is a diffeomorphic transformation for positive reals.

2.7 Julia implementation of higher-order approximations

One is often confronted with challenges when translating mathematical ideas into executable software. Edgeworth series in particular are simple in their mathematical definition, but hide the use of many mathematical concepts that, independently, are commonly cumbersome to translate into easy-to-use and bug-free software. A generic implementation of Edgeworth series requires the ability to compute derivatives, express and manipulate asymptotic expansions and combine those to create density approximations.

Luckily, modern programming languages and libraries allow to quickly develop algorithms that are both efficient and close to their mathematical counterpart. In this thesis, we make use of the Julia programming language [8], and Julia bindings to the computer algebra system SymPy [24]. The Julia programming language was chosen because it allows to write code that is generic enough to be used in various scenarios and extended with the ecosystem of libraries. For instance, one building block of the approximations developed in this thesis is the cumulant generating function of a distribution. The cumulant generating function of a $\Gamma(\alpha, \beta)$ distribution can be defined as the function

```
julia> gamma(p, λ) = t -> p*log(λ) - p*log(λ-t)
```

This function can then both be used with concrete values of p, λ and t, for instance $\text{gamma}(1.0, 2.0)(1.0) = 0.6931471805599453$. However, one can also define symbolic variables for p and λ to construct a symbolic expression of the cumulant generating function

```
julia> @syms p::positive λ::positive
julia> gamma(p, λ)(1.0)
p*log(λ) - p*log(λ-1.0)
```

This modularity can be used to construct helper functions to manipulate cumulant generating functions based on other libraries. For instance, if we are interested in computing the cumulants of a distribution, we can use the same definition of the cumulant function and use the TaylorSeries [7] library to efficiently compute the derivatives of the cumulant generating function. This let's us define the following function to compute the first n cumulants of a distribution from its cumulant generating function

```
function cumulants(K, n; T=Number)
    t = Taylor1(T, n+1)
    (K(t).coeffs ./ exp(t).coeffs)[2:end]
end
```

Julia's extensibility makes it easy to combine several libraries to develop more advanced functionalities. For instance, the code presented above can be used to compute the generic formula of the mean and variance of a $\Gamma(p, \lambda)$ distribution without having to program the interaction between Julia's SymPy bindings and the TaylorSeries library

```
julia> @syms p::positive λ::positive
julia> μ, σ^2 = cumulants(gamma(p, λ), 2)
2-element Vector{Sym}:
   p/λ
   p/λ^2
```

We used the capability of Julia to compose high-level libraries in order to develop a generic procedures for manipulating cumulant generating functions and develop density approximations for sums and maximum likelihood estimators. As an example, Listing 1 implements an arbitrary-order Edgeworth expansion by combining the mathematical derivation of the Edgeworth series in Section 2.2 and some of the ideas described above.

A particularly appealing example of the usage of the function in Listing 1 is to derive the generic formula of the Edgeworth series of a specific order given the required cumulants. We start by defining a function `symcgf(cumulants)` which creates a cumulant generating function with cumulants provided as an argument. For instance,

```
julia> @syms t::real κ3::real κ4::real
julia> K = symcgf([0.0; 1.0; κ3; κ4])
julia> cumulants(K, 5; T=Sym)
5-element Vector{Sym}:
 0
 1
 κ3
 κ4
 0
```

We can then use the `edgeworth` from Listing 1 to compute the explicit formula for the Edgeworth series of order 4[2]

[2]To avoid writing out the Hermite polynomials, we use a sligthly modified version of the code in Listing 1 replacing Hermite polynomials by symbolic functions H_k.

```
julia> edgeworth(K, n, 4; T=Sym)(x)
```

$$0.398942280401433\left(1 + \frac{\kappa_3^2 H_6(x)}{72n} + \frac{\kappa_4 H_4(x)}{24n} + \frac{\kappa_3 H_3(x)}{6\sqrt{n}}\right) e^{\frac{-x^2}{2}}$$ [3]

With $(2\pi)^{-1/2} \approx 0.398942280401433$, this formula corresponds expression derived in (2.12) of Example 2.7.

Listing 1: Symbolic implementation of the Edgeworth expansion

```
function edgeworth(K, nsum, order; T=Float64)
    H(k) = basis(ChebyshevHermite, k)
    finaltype = promote_rule(T, typeof(nsum))
    taylororder = 3*order+1

    # Define two symbolic variables t and n. We use t as
    # variable  of the cgf for computing Taylor series and
    # n as the symbolic number of elements in the sum in
    # order to be able to track terms of various orders of n.
    @vars t n::(positive, integer)

    # Start by constructing the cgf of ∑(X_i - μ)/√(σ²n),
    # as discussed in Remark 2.8.
    μ, σ² = cumulants(K, 2; T=T)
    stdK = affine(K, -μ, 1/sqrt(σ²*n))
    sumK = iidsum(stdK, n)

    # Use the new cgf to construct the expansion of the ratio
    # of characteristic functions, as in (2.6).
    ratio = exp(sumK(t) - t^2/2)
    expansion = ratio.series(t, n=taylororder).removeO()

    # Then proceed by truncating the expansion to the desired
    # order and replace the symbolic n by its true value.
    expansion = collect(expand(expansion), n)
    expansion = truncate_order(expansion, n, (1-order)/2)
```

[3] This output was lightly adapted to properly render in LaTeX.

```
    expansion = subs(expand(expansion), n, nsum)

    # The ‘expansion‘ variable is now a symbolic polynomial
    # in the variable t. We retrieve the density by Fourier
    # inversion, by which we replace instances of t^k by the
    # k–th Hermite polynomial as in (2.8).
    αstar = collect(expansion, t).coeff.(t.^(0:taylororder))
    αstar = convert.(finaltype, αstar)
    polynomial = sum([αstar[i]*H(i-1) for i=1:length(αstar)])

    # Finally, the approximate density can be constructed
    # as done in 2.8 and using Remark 2.8.
    function density(z)
        κ1 = sqrt(nsum)*μ; x = (z - κ1) / sqrt(σ^2)
        return exp(-x^2/2)/sqrt(σ^2*2π) * polynomial(x)
    end
end
```

3 Gaussian Graphical Models

In this chapter, we study problems related to submodel selection in Gaussian graphical models. In Section 3.1, we begin by defining graphical models and Gaussian graphical models. We then study the existence and computation of the maximum likelihood estimator of the precision matrix in a Gaussian graphical model under different assumptions on the graph. In Section 3.3, we apply the p^* approximation from Section 2.6 to compute an accurate approximation for submodel testing. The test resulting from this approximation is then numerically evaluated against the likelihood ratio test in different dimensionality settings.

3.1 Preliminaries

We begin with a brief introduction to elementary concepts in graph theory. Let $\mathcal{G} = (\Gamma, E)$ be a graph with nodes Γ and edges E. In the sequel, we only consider unconnected and loopless graphs. For notational simplicity, we assume that the nodes Γ are numbered. For $p = |\Gamma|$, we write $\mathcal{G} = ([p], E)$ and have that $E \subset \{\{i, j\} : i, j \in [p], i \neq j\}$. If $e = \{i, j\} \in E$ for some $i, j \in [p]$, we call i and j *endpoints* of e and write $i, j \in e$. We denote by $\mathrm{bd}(i)$ the set of *neighbours* of $i \in [p]$, that is $\mathrm{bd}(i) = \{j \in [p] : \{i, j\} \in E \text{ and } j \neq i\}$. Note that it will be useful to treat the set of edges as a set of indices on a matrix. For this case, we introduce the *augmented edge set*, in order to include indices refering to the diagonal entries of a matrix. The augmented edge set E^* of E is the set $E^* = E \cup \{\{i\} : i \in \Gamma\}$, constructed by adding all possible loops in $\mathcal{G}$.

A graph $\mathcal{G}$ is said to be *complete* if all pairs of distinct nodes are connected by an edge. A *clique* of $\mathcal{G}$ is a set of nodes $C \subset [p]$ such that the subgraph $\mathcal{G}_C = (C, E_C)$ with $E_C = \{\{i, j\} \in E : \{i, j\} \subset C\}$ is complete. We denote by $\mathcal{C}(\mathcal{G})$ the set of cliques in $\mathcal{G}$. Let $l \in \mathbb{N}$, a *l-cycle* is a set of nodes $i_1, \ldots, i_l \in [p]$ such that $\{i_j, i_{j+1}\} \in E$ for $j \in [l]$ and $\{i_1, i_l\} \in E$. A *chord* is an edge e connecting two nodes of a cycle that is not part of the cycle. A *chordless cycle* is a cycle which has no chord. A *chordal graph* $\mathcal{G}$ is a graph which contains no chordless cycle of length greater or equal to 4.

Let $\mathcal{G} = ([p], E)$ and $M \in \mathbb{R}^{p \times p}$. We introduce the following notation.

- If $e = \{i, j\} \in E$, then $M_e = M_{ij}$.
- If $A, B \subset [p]$, then $M_{A,B}$ is the $|A| \times |B|$ matrix constructed by keeping rows labeled by the entries in A and columns labeled by the entries in B.
- If $A \subset [p]$, then $M_A = M_{A,A}$.

- If $A, B \subset [p]$, then $[M_{A,B}]^{[p]}$ is the $p \times p$ matrix with entries given by

$$[M_{A,B}]^{\Gamma}_{ij} = \begin{cases} M_{ij} & \text{if } \{i,j\} \in A \times B, \\ 0 & \text{otherwise.} \end{cases}$$

Since most matrices manipulated in this thesis reference quantities related to nodes in a graph, we index matrices with respect to the nodes of the graph instead of row or column number of the matrix. For instance, if $A, B \subset [p]$ and $M \in \mathbb{R}^{p \times p}$, then following the notation introduced above, we have that

$$(M_{A,B})_{ab} = M_{ab} \quad \text{for all } a \in A, b \in B.$$

We denote by $\mathcal{S}^p$ the set of $p \times p$ symmetric matrices and $\mathcal{S}^p_{\succ 0}$ the set of $p \times p$ positive definite symmetric matrices. Let $\mathcal{G} = ([p], E)$, we define the set of matrices $\mathcal{S}(\mathcal{G}) = \{M \in \mathcal{S}^p : M_e = 0 \text{ if } e \notin E^*\}$ and $\mathcal{S}_{\succ 0}(\mathcal{G}) = \{M \in \mathcal{S}(\mathcal{G}) : M \text{ is positive definite }\}$ or equivalently $\mathcal{S}_{\succ 0}(\mathcal{G}) = \mathcal{S}(\mathcal{G}) \cap \mathcal{S}^p_{\succ 0}$.

3.2 Maximum likelihood estimation in Gaussian graphical models

A graphical model is a probabilistic model associating relations between random variables to a graph. The random variables of the model are represented by nodes in the graph and conditional independence relations are represented by missing edges between the corresponding nodes of the graph.

Consider a random vector X distributed according to the *multivariate Gaussian distribution* $N_p(0, \Omega^{-1})$, where the *precision matrix* $\Omega \in \mathcal{S}^p_{\succ 0}$ is the inverse of the covariance matrix Σ. Thus, the density of X is

$$f(x; \Omega) = (2\pi)^{-p/2} |\Omega|^{1/2} \exp\left\{ -\frac{1}{2} \text{tr}\left[x x^\top \Omega \right] \right\}. \tag{3.1}$$

Clearly, the multivariate Gaussian distribution is an exponential family with canonical parameter Ω and sufficient statistic $\frac{1}{2} x x^\top$. We start by stating a result about multivariate Normal distributions that can be found in [21, Proposition C.5].

Lemma 3.1. Let $X \sim N_p(\mu, \Sigma)$ and $A, B \subset [p]$ be disjoint. Then, the conditional

distribution of X_A given $X_B = x_B$ is $N_{|A|}(\mu_{A|B}, \Sigma_{A|B})$ where

$$\mu_{A|B} = \mu_A + \Sigma_{A,B}\Sigma_{B,B}^{-1}(x_B - \mu_B) \qquad \text{and} \qquad \Sigma_{A|B} = \Sigma_{A,A} - \Sigma_{A,B}\Sigma_{B,B}^{-1}\Sigma_{B,A}.$$

One recognizes that the conditional covariance matrix $\Sigma_{A|B}$ is the Schur complement of Σ_B in Σ.

We parametrize the multivariate Normal distribution in terms of the precision matrix because of its special role in the context of graphical models. Indeed, the conditional independence relations of the entries a random vector $X \sim N_p(0, \Omega)$ are characterized by the sparsity patterns of the precision matrix Ω. This is shown in the following lemma from [21, Proposition 5.2].

Lemma 3.2. Let $X \sim N_p(\mu, \Sigma)$ and let $i, j \in [p]$ with $i \neq j$. Then

$$\Omega_{ij} = 0 \iff X_i \perp\!\!\!\perp X_j | X_{[p]\setminus\{i,j\}}. \tag{3.2}$$

Proof. By Lemma 3.1, we have that the bivariate vector $X_{\{i,j\}}$ is Gaussian with covariance matrix $\Sigma_{\{i,j\}|[p]\setminus\{i,j\}}$ equal to the Schur complement of $\Sigma_{[p]\setminus\{i,j\}}$. The statement in (3.2) is thus equivalent to

$$\Omega_{ij} = 0 \iff \Sigma_{\{i,j\}|[p]\setminus\{i,j\}} \text{ is diagonal.}$$

Using the Schur complement inverse property, we have that

$$\Sigma_{\{i,j\}|[p]\setminus\{i,j\}} = \left[\Omega_{\{i,j\}}\right]^{-1} = \begin{pmatrix} \Omega_{ii} & \Omega_{ij} \\ \Omega_{ji} & \Omega_{jj} \end{pmatrix}^{-1} = \frac{1}{|\Omega_{\{i,j\}}|} \begin{pmatrix} \Omega_{jj} & -\Omega_{ij} \\ -\Omega_{ji} & \Omega_{ii} \end{pmatrix}^{-1}.$$

Hence, $\Sigma_{\{i,j\}|[p]\setminus\{i,j\}}$ is diagonal if and only if $\Omega_{ij} = 0$, completing the proof of the lemma. □

Consider a graph $\mathcal{G} = ([p], E)$. We say that X satisfies the *Gaussian graphical model* with graph $\mathcal{G}$ if $X \sim N_p(0, \Omega)$ and

$$\Omega_{ij} = 0 \text{ for all } \{i, j\} \notin E^*. \tag{3.3}$$

Property (3.3) corresponds to the pairwise Markov property in graphical model theory [21]. Note that the independence relations of the entries of X, the connectivity of the nodes in $\mathcal{G}$ and the sparsity pattern of Ω are all the same concept viewed from a different angle, which each on its own will help in studying them.

We now study properties of the maximum likelihood estimator in a Gaussian graphical model, largely the presentation of Uhler [23, Section 9].

Consider a sample $X = (X_1, \ldots, X_n)$ from a Gaussian distribution. The log-likelihood function for a precision matrix $\Omega \in \mathcal{S}^p_{\succ 0}$ obtained from (3.1) is

$$\ell(\Omega; X) = \frac{n}{2} \log |\Omega| - \frac{1}{2} \mathrm{tr}[XX^\top \Omega].$$

Rewriting the log-likelihood in terms of the sufficient statistic $S = n^{-1} XX^\top$, we get that

$$\ell(\Omega; S) = \frac{n}{2} \log |\Omega| - \frac{n}{2} \mathrm{tr}[S\Omega]. \tag{3.4}$$

In the *saturated model* where no constraints are put on the entries of Ω, the maximum likelihood estimator is defined when $S \in S^p_{\succ 0}$ and is equal to

$$\hat{\Omega} = S^{-1}.$$

Note that, if we are interested in estimating the maximum likelihood estimator $\hat{\Omega}$ of a Gaussian graphical model with graph $\mathcal{G} = ([p], E)$, the solution $\hat{\Omega}$ must lie in the subset $\mathcal{S}_{\succ 0}(\mathcal{G})$ of $\mathcal{S}^p_{\succ 0}$ in which the conditional independence relations encoded in $\mathcal{G}$ are satisfied. We are left with the following optimization problem

$$\begin{aligned} &\underset{\Omega \in \mathcal{S}^p_{\succ 0}}{\text{maximize}} \quad \log |\Omega| - \mathrm{tr}[S\Omega] \\ &\text{subject to} \quad \Omega \in \mathcal{S}(\mathcal{G}). \end{aligned} \tag{3.5}$$

Since the Gaussian graphical model condition is a linear constraint, the set $\mathcal{S}(\mathcal{G})$ is a convex cone. Showing that the objective function in (3.5) is concave would imply that maximum likelihood estimation in Gaussian graphical models is a convex optimization problem. This would allow us to bring new insights to the maximum likelihood problem by studying its dual formulation. The following lemma from [23, Proposition 9.2.1] states that the objective function is indeed concave.

Lemma 3.3. The function $f : \mathcal{S}^p_{\succ 0} \to \mathbb{R}, X \mapsto \log |X| - \mathrm{tr}\,[SX]$ is concave.

Proof. Remark that the sum of a concave function and a linear function is concave, and $\mathrm{tr}\,[SX]$ is linear in X. Thus, it is sufficient to show that the logarithm of the determinant of a matrix is concave. To show this, we consider the line $\{U + tV : t \in \mathbb{R}\}$ for $U, V \in \mathcal{S}^p_{\succ 0}$. We show that $X \mapsto \log |X|$ is concave on $\mathcal{S}^p_{\succ 0}$ by proving that $g(t) = \log |U + tV|$ is concave

as follows. Since $U \in \mathcal{S}^p_{\succ 0}$, both $U^{1/2}$ and $U^{-1/2}$ exist and we have

$$\begin{aligned} g(t) &= \log|U + tV| \\ &= \log|U^{1/2}(1_p + tU^{-1/2}VU^{-1/2}| \\ &= \log|U| + \log|1_p + tU^{-1/2}VU^{-1/2}|. \end{aligned}$$

Let λ_i be the eigenvalues of $U^{-1/2}VU^{-1/2}$ and note that the eigenvalues of $1_p + tU^{-1/2}VU^{-1/2}$ are $1 + t\lambda_i$. Therefore

$$g(t) = \log|U| + \sum_{i=1}^{p} \log(1 + t\lambda_i).$$

Now, since each $\log(1 + t\lambda_i)$ is concave in t, we have that g is concave, which completes the proof of the lemma. □

We can now study the dual problem to (3.5). The Lagrangian of the likelihood maximization problem in Gaussian graphical models is given by

$$\begin{aligned} \mathcal{L}(\Omega, \nu) &= \log|\Omega| - \operatorname{tr}[S\Omega] - 2 \sum_{\{i,j\} \notin E} \nu_{ij}\Omega_{ij} \\ &= \log|\Omega| - \sum_{i=1}^{p} S_{ii}\Omega_{ii} - 2 \sum_{\{i,j\} \in E} S_{ij}\Omega_{ij} - 2 \sum_{\{i,j\} \notin E} \nu_{ij}\Omega_{ij} \end{aligned}$$

The Lagrange dual H of (3.5) is given by $H(\nu) = \mathcal{L}(\Omega^\nu, \nu)$ where Ω^ν is the maximizer of $\mathcal{L}(\Omega, \nu)$. Let Ω^ν be the maximizer of $\mathcal{L}(\Omega, \nu)$ with respect to Ω. Then, finding the roots Ω^ν_{ij} of $\frac{\mathrm{d}}{\mathrm{d}\Omega_{ij}}\mathcal{L}(\Omega, \nu)$ shows that the inverse Σ^ν of Ω^ν satisfies the following

$$\Sigma^\nu_{ij} = \begin{cases} S_{ij} & \text{if } i = j \text{ or } \{i,j\} \in E, \\ \nu_{ij} & \text{otherwise.} \end{cases}$$

Note that Σ^ν is the matrix formed by replacing entries in S corresponding to missing edges with entries of the dual variables ν_{ij}. Replacing Ω^ν in the expression for the Lagrange

dual function H, we obtain that

$$\begin{aligned} H(\nu) = \mathcal{L}(\Omega^\nu, \nu) &= \log|\Omega^\nu| - \operatorname{tr}[S\Omega^\nu] - 2\sum_{\{i,j\}\notin E} \nu_{ij}\Omega^\nu_{ij} \\ &= \log|\Omega^\nu| - \operatorname{tr}[\Sigma^\nu\Omega^\nu] + 2\sum_{\{i,j\}\notin E} \Sigma^\nu_{ij}\Omega^\nu_{ij} - 2\sum_{\{i,j\}\notin E} \nu_{ij}\Omega^\nu_{ij} \\ &= \log|\Omega^\nu| - p = -\log|\Sigma^\nu| - p. \end{aligned}$$

Hence, the dual to (3.5) is

$$\begin{aligned} &\underset{\Sigma\in\mathcal{S}^p_{\succ 0}}{\text{minimize}} \quad -\log|\Sigma| - p \\ &\text{subject to} \quad \Sigma_{ij} = S_{ij} \quad \text{for all } \{i,j\} \in E^*. \end{aligned} \tag{3.6}$$

To prove that problems (3.5) and (3.6) are equivalent, we must show that strong duality holds for this convex optimization problem. By *Slater's constraint quantification* [9, Section 5.3.2], it is enough to show that there exists an $\Omega^* \in \mathcal{S}^p_{\succ 0}$ that is strictly feasable for the primal problem. Since the identity matrix is positive definite and is an element of $\mathcal{S}(\mathcal{G})$ for any $\mathcal{G}$, strong duality holds for any graph $\mathcal{G}$. Thus, we can freely study both formulations of the optimization problem. Furthermore, Problems (3.5) and (3.6) have a solution if and only if $\log|\Sigma| + p$ is bounded from above in the set of feasable matrices. We have yet to study under which condition this is the case.

To that end, let us first introduce some notation. Let $\mathcal{G} = ([p], E)$ and let $\Sigma \in \mathbb{R}^{p\times p}$, the *$\mathcal{G}$-partial matrix* $\Sigma^\mathcal{G}$ of Σ is the partial matrix constructed by removing entries in Σ corresponding to missing edges in $\mathcal{G}$, see Figure 5 for an example. With this notation, the dual problem (3.6) can be reformulated as follows,

$$\begin{aligned} &\underset{\Sigma\in\mathcal{S}^p_{\succ 0}}{\text{minimize}} \quad -\log|\Sigma| - p \\ &\text{subject to} \quad \Sigma^\mathcal{G} = S^\mathcal{G}. \end{aligned} \tag{3.7}$$

In this formulation, the dual optimization problem corresponds to a *positive definite matrix completion* problem in which the matrix Σ is partially specified from entries of the sample covariance matrix corresponding to edges present in $\mathcal{G}$. Furthermore, Uhler [23, Section 9.4] presents a geometric argument tying together the matrix completion to the original convex optimization formulation of the likelihood maximization problem. We state without a proof a reformulation of [23, Theorem 9.4.2], in which we use that $\mathcal{L} \cap \mathcal{S}^p_{\succ 0} = \mathcal{S}(\mathcal{G})$, which we have shown to contain at least 1_p.

Theorem 3.4. Consider a Gaussian graphical model associated to the graph $\mathcal{G}$ and a sample covariance matrix S. The likelihood maximization primal and dual problems have unique solutions $\hat{\Omega}$ and $\hat{\Sigma}$ if and only if $S^{\mathcal{G}}$ has a positive definite completion. In this case, $\hat{\Sigma}$ is the positive definite completion of $S^{\mathcal{G}}$ and $\hat{\Omega} = \hat{\Sigma}^{-1}$.

We now study the existence of a solution to the maximum likelihood question by finding the conditions under which a $\mathcal{G}$-partial sample covariance matrix can be completed to a positive definite matrix. Gross et al. [18] introduce the *maximum likelihood threshold* of a graph $\mathcal{G}$. The maximum likelihood treshold of a graph $\mathcal{G}$, denoted by $\text{mlt}(\mathcal{G})$, is the smallest sample size guaranteeing that the maximum likelihood estimator exists almost surely in a Gaussian graphical model associated to the graph $\mathcal{G}$. In other words, $\text{mlt}(\mathcal{G})$ is the smallest number of observations for which $S^{\mathcal{G}}$ can be almost surely completed to a positive definite matrix. For a Gaussian graphical model over p variables, the rank of the sample covariance constructed from a sample of n observations is almost surely $\text{rank}(S) = \min(n, p)$. Hence, if $n \geq p > 0$, S itself is a valid positive completion of $S^{\mathcal{G}}$, giving the worst case bound

$$\text{mlt}(\mathcal{G}) \leq p, \tag{3.8}$$

where equality holds if $\mathcal{G}$ is complete.

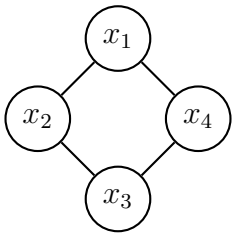
A necessary condition for a solution to the matrix completion problem to exist is that all completely specified principal submatrices $S^{\mathcal{G}}_{[p]\setminus I}$ of $S^{\mathcal{G}}$ for $I \subset [p]$ must be positive definite. The principal submatrix $S^{\mathcal{G}}_{[p]\setminus I}$ of $S^{\mathcal{G}}$ is completely specified if it contains no missing value. The necessary condition can be shown by the following argument. Let $S^{\mathcal{G}}_{[p]\setminus I}$ be a principal completely specified submatrix of $S^{\mathcal{G}}$ such that there exists $z \in \mathbb{R}^{p-|I|} \setminus \{0\}$ with $z^\top S^{\mathcal{G}}_{-I} z \leq 0$. Then if $S^{\mathcal{G}}_{+}$ is the positive definite completion of $S^{\mathcal{G}}$, it holds that $x^\top S^{\mathcal{G}}_{+} x \leq 0$ for $x \in \mathbb{R}^p \setminus \{0\}$ with $x_I = z$ and $x_{[p]\setminus I} = 0$, contradicting the positive definiteness of $S^{\mathcal{G}}_{+}$. Furthermore, if C is a clique of $\mathcal{G}$, C is complete and thus the submatrix $S^{\mathcal{G}}_{C}$ is a completely specified principal submatrix of $S^{\mathcal{G}}$. As $S^{\mathcal{G}}_{C}$ is complete, it is positive definite with probability one if and only if $n \geq |C|$. Now let $q(\mathcal{G}) = \max\{|C| : C \text{ is a clique of } \mathcal{G}\}$ be the maximum clique size in $\mathcal{G}$. We can lower bound the maximum likelihood threshold by

$$q(\mathcal{G}) \leq \text{mlt}(\mathcal{G}). \tag{3.9}$$

However, as shown in the example in Figure 5, this condition is not sufficient for the existence of a positive definite completion. Still, Grone et al. [17] show that this condition is also sufficient if and only if $\mathcal{G}$ is a chordal graph.

$$\begin{pmatrix} 1 & 0.9 & 0.3 & -0.9 \\ 0.9 & 1 & 0.9 & -0.7 \\ 0.3 & 0.9 & 1 & 0.9 \\ -0.9 & -0.7 & 0.9 & 1 \end{pmatrix}$$

S



$$\begin{pmatrix} 1 & 0.9 & ? & -0.9 \\ 0.9 & 1 & 0.9 & ? \\ ? & 0.9 & 1 & 0.9 \\ -0.9 & ? & 0.9 & 1 \end{pmatrix}$$

$S^{\mathcal{G}}$

Figure 5: Example from [23, Section 9.3] of a matrix S for which all completely specified submatrices of $S^{\mathcal{G}}$ are positive definite but where S doesn't have a positive definite completion.

Theorem 3.5. For a graph $\mathcal{G}$, the following statements are equivalent.

i. A partial matrix $M^{\mathcal{G}}$ has a positive definite completion if and only if all completely specified submatrices of $M^{\mathcal{G}}$ are positive definite.

ii. $\mathcal{G}$ is chordal.

A consequence of this theorem is that if $\mathcal{G}$ is a chordal graph, then $\text{mlt}(\mathcal{G}) = q(\mathcal{G})$. This result for chordal graphs can be used to compute an upper bound on the maximum likelihood treshold of a general graph, tighter than the worst-case bound in (3.8).

Let $\mathcal{G} = (\Gamma, E)$ be a graph and S a sample covariance matrix. A graph $\mathcal{G}^+ = (\Gamma, E^+)$ is called a *chordal cover* of $\mathcal{G}$ if $E \subset E^+$ and $\mathcal{G}^+$ is chordal. Then, since $E \subset E^+$, we have that the $\mathcal{G}^+$-partial matrix $S^{\mathcal{G}^+}$ agrees with the $\mathcal{G}$-partial matrix $S^{\mathcal{G}}$ on the entries corresponding to the edges E of $\mathcal{G}$. Thus, one can view $S^{\mathcal{G}^+}$ as a partial completion of $S^{\mathcal{G}}$, and any positive definite completion of $S^{\mathcal{G}^+}$ is a valid positive completion of $S^{\mathcal{G}}$. Hence, by Theorem 3.5, the following bound holds

$$\text{mlt}(\mathcal{G}) \leq q^+(\mathcal{G}) = \min\left\{q(\mathcal{G}^+) : \mathcal{G}^+ \text{ is a chordal cover of } \mathcal{G}\right\}.$$

Combining (3.9) and the above bound, it follows that for any graph $\mathcal{G}$,

$$q(\mathcal{G}) \leq \text{mlt}(\mathcal{G}) \leq q^+(\mathcal{G}). \tag{3.10}$$

Example 3.6. Let $\mathcal{G} = ([p], E)$ be a chordless cycle of length $p \geq 4$, $E = \{\{1,2\},\{2,3\},\ldots,\{p,1\}\}$. Then, the maximal clique size of $\mathcal{G}$ is $q(\mathcal{G}) = 2$. We can form a chordal cover $\mathcal{G}^+ = ([p], E^+)$ that attains the minimum $q(\mathcal{G}^+) = 3$ by connecting an arbitrary node $a \in [p]$ to all other nodes of $\mathcal{G}$ that are not already neighbours of a. That is, we define the set of edges of $\mathcal{G}^+$ by $E^+ = E \cup \{\{a,i\} : i \in [p] \setminus \{a\}\}$. This chordal

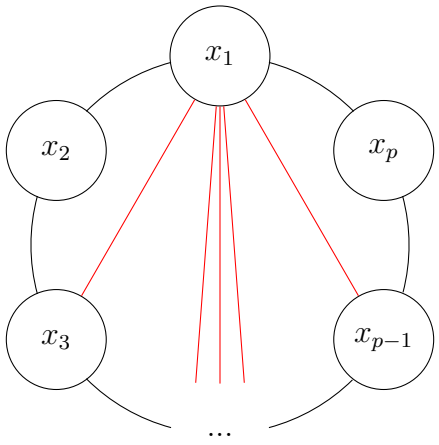


Figure 6: The graph $\mathcal{G} = ([p], E)$ formed from the black edges in the above figure is a cycle of length p. If E^+ is formed by adding the red edges in the figure to E, then $\mathcal{G}^+ = ([p], E^+)$ forms a chordal cover of $\mathcal{G}$.

covering is depicted in Figure 6, with $a = 1$. Hence, for a chordless cycle $\mathcal{G}$ of size p,

$$2 \leq \text{mlt}(\mathcal{G}) \leq 3.$$

The exact conditions under which the maximum likelihood estimator in a chordless cycle exists for $n = 2$ are studied in Buhl [10, Section 4].

Now that we have presented some of the conditions under which one can almost surely find a positive definite completion to the $\mathcal{G}$-partial correlation matrix $S^{\mathcal{G}}$, we turn ourselves to the question of finding an algorithm capable of computing the maximum likelihood estimator $\hat{\Sigma}$ of Σ. As discussed earlier, the completely specified principal submatrices of $S^{\mathcal{G}}$ are the submatrices corresponding to the cliques of $\mathcal{G}$. Hence, finding a positive definite completion of $\mathcal{S}^{\mathcal{G}}$ is equivalent to finding the matrix $\hat{\Sigma}$ satisfying for all $C \in (C)(\mathcal{G})$,

$$\hat{\Sigma}_C = S_C. \tag{3.11}$$

This equation naturally suggests an iterative algorithm by successively adjusting parts of the covariance matrix to satisfy (3.11) while keeping the running matrix positive definite. This procedure, called *iterative proportional scaling*, was studied by Speed and Kiiveri [26], among with other algorithms for solving the maximum equation problem in Gaussian graphical models.

Next, we present a development of the algorithm in a Gaussian graphical model with graph $\mathcal{G}$, given a sample covariance matrix C computed from a sample of size $n > \text{mlt}(\mathcal{G})$.

Let $\Omega \in \mathcal{S}^p_{\succ 0}$ be a positive definite matrix and let $C \in \mathcal{C}(\mathcal{G})$ be a clique of $\mathcal{G}$. We define the *C-marginal adjustment* operator T_C given by

$$T_C\Omega = \Omega + \begin{pmatrix} (S_C)^{-1} - (\Sigma_C)^{-1} & 0 \\ 0 & 0 \end{pmatrix}, \tag{3.12}$$

where the variable Σ denotes the inverse of Ω, and for simplicity of notation, the top-left block of matrices writen out explicitly corresponds to the current clique C. We now show that the operator T_C satisfies the following useful properties.

Proposition 3.7. Let $\mathcal{G} = ([p], E)$ and S be an empirical covariance matrix constructed from a sample of size $n > \text{mlt}(\mathcal{G})$ from the Gaussian graphical model associated to $\mathcal{G}$. Then, the operator T_C satisfies the following properties.

i. T_C is well defined;

ii. T_C adjusts the C-marginal of Ω. That is, $(T_C\Omega)^{-1}$ satisfies (3.11) for the clique C;

iii. If $\Omega \in \mathcal{S}^p_{\succ 0}$, then $T_C\Omega \in \mathcal{S}^p_{\succ 0}$;

iv. If $\Omega \in \mathcal{S}(\mathcal{G})$, then $T_C\Omega \in \mathcal{S}(\mathcal{G})$.

Proof. (i) By assumption on the sample size n, all matrices and submatrices involved in T_C are positive definite and can be inverted.
(ii) As seen earlier, the inverse of Σ_C can be expressed in terms of Ω by using the Schur complement

$$(\Sigma_C)^{-1} = \Omega_C - \Omega_{C,C^c}(\Omega_{C^c})^{-1}\Omega_{C^c,C},$$

where $C^c = [p] \setminus C$ is the complement of C in $[p]$. Replacing this in the definition of T_C gives

$$T_C\Omega = \begin{pmatrix} (S_C)^{-1} + \Omega_{C,C^c}(\Omega_{C^c})^{-1}\Omega_{C^c,C} & \Omega_{C,C^c} \\ \Omega_{C^c,C} & \Omega_{C^c,C^c} \end{pmatrix}. \tag{3.13}$$

We can now use the Schur complement to compute the C-marginal of Ω,

$$\begin{aligned} \left[(T_C\Omega)^{-1}\right]_C &= \left[(S_C)^{-1} + \Omega_{C,C^c}(\Omega_{C^c})^{-1}\Omega_{C^c,C} - \Omega_{C,C^c}(\Omega_{C^c})^{-1}\Omega_{C^c,C}\right]^{-1} \\ &= \left[(S_C)^{-1}\right]^{-1} = S_C. \end{aligned}$$

(iii) In [21, Proposition B.1], Lauritzen gives a sufficient condition for a symmetric diagonal to be positive definite. Applying this proposition, we have that $T_C\Omega$ is positive definite if and only if both $(T_C\Omega)_C$ and $E = (T_C\Omega)_C - (T_C\Omega)_{C,C^c}((T_C\Omega)_{C^c})^{-1}(T_C\Omega)_{C^c,C}$ are positive definite. As seen in (ii), $(T_C\Omega)_C = S_C$ is by assumption positive definite. As for the Schur

Algorithm 1 Iterative proportional scaling

Input: Set of cliques $\mathcal{C}(\mathcal{G})$, sample covariance matrix S, tolerance ε.
Output: Maximum likelihood estimator $\hat{\Omega}$.

1: Let $\Omega^0 = 1_p$
2: Let $\Omega^1 = \Omega^0$
3: **for** $C \in \mathcal{C}(\mathcal{G})$ **do**
4: Set $\Omega^1 := T_C\Omega^1$
5: **end for**
6: **if** $\|\Omega^1 - \Omega^0\| < \varepsilon$ **then**
7: Return $\hat{\Omega} := \Omega^1$
8: **else**
9: Set $\Omega^0 := \Omega^1$
10: Go to line 2.
11: **end if**

complement,

$$\begin{aligned} E &= (T_C\Omega)_C - (T_C\Omega)_{C,C^c}((T_C\Omega)_{C^c})^{-1}(T_C\Omega)_{C^c,C} \\ &= (S_C)^{-1} + \Omega_{C,C^c}(\Omega_{C^c})^{-1}\Omega_{C^c,C} - \Omega_{C,C^c}(\Omega_{C^c})^{-1}\Omega_{C^c,C} \\ &= (S_C)^{-1}, \end{aligned}$$

is by the same assumption positive definite. Hence $T_C\Omega$ is positive definite.
(iv) Let E be the set of edges of $\mathcal{G}$ and $e = \{i, j\} \notin E$ be a missing edge in $\mathcal{G}$. Since C is a clique of $\mathcal{G}$, we have that $|C \cap \{i, j\}| \leq 1$ and the entry of the matrix $T_C\Omega$ corresponding to the edge $\{i, j\}$ is in one of the following submatrices: $(T_C\Omega)_{C,C^c}$, $(T_C\Omega)_{C^c}$ or $(T_C\Omega)_{C^c,C}$. Since these submatrices are left invariant under T_C, we have that $(T_C\Omega)_{ij} = \Omega_{ij} = 0$, thus $T_C\Omega \in \mathcal{S}(\mathcal{G})$. □

Given these properties, we can naturally define an algorithm by cycling through the cliques $C \in \mathcal{C}(\mathcal{G})$ of $\mathcal{G}$, successively adjusting each C-marginal by applying the adjustment operator T_C, and repeating until convergence. This algorithm is the iterative proportional scaling algorithm, given in Algorithm 1. The question remains of whether this algorithm converges and why. We start by showing that the C-marginal adjustment operator computes the solution to a constrained version of (3.5). A proof of this lemma can be found within the proof of [21, Theorem 5.4].

Lemma 3.8. Let $\Omega^0 \in \mathcal{S}_{\succ 0}(\mathcal{G})$. The C-marginal adjustment operator T_C computes the solution to problem (3.5) over the section

$$\Theta_C(\Omega^0) = \left\{\Omega \in \mathcal{S}_{\succ 0}(\mathcal{G}) : \Omega_{C^c} = \Omega^0_{C^c} \text{ and } \Omega_{C,C^c} = \Omega^0_{C,C^c}\right\}.$$

That is, $T_C\Omega^0$ is the solution to

$$\begin{aligned} &\underset{\Omega \in \mathcal{S}_{\succ 0}(\mathcal{G})}{\text{maximize}} && \log|\Omega| - \operatorname{tr}[S\Omega] \\ &\text{subject to} && \Omega_{C^c} = \Omega^0_{C^c} \text{ and } \Omega_{C,C^c} = \Omega^0_{C,C^c}. \end{aligned} \tag{3.14}$$

Proof. Using the expression of the determinant of a block matrix in terms of Schur complement, we have that

$$|\Omega| = \left|\Omega_C - \Omega_{C,C^c}(\Omega_{C^c})^{-1}\Omega_{C^c,C}\right| |\Omega_{C^c}|.$$

Furthermore, using the fact that $\Omega \in \Theta(\Omega^0)$, it follows that

$$\begin{aligned} \log|\Omega| &= \log\left\{\left|\Omega_C - \Omega^0_{C,C^c}(\Omega^0_{C^c})^{-1}\Omega^0_{C^c,C}\right| \left|\Omega^0_{C^c}\right|\right\} \\ &= \log\left|\Omega_C - \Omega^0_{C,C^c}(\Omega^0_{C^c})^{-1}\Omega^0_{C^c,C}\right| + \log\left|\Omega^0_{C^c}\right| \\ &= \log|\Omega'| + \log\left|\Omega^0_{C^c}\right|, \end{aligned}$$

where $\Omega' = \Omega_C - \Omega^0_{C,C^c}(\Omega^0_{C^c})^{-1}\Omega^0_{C^c,C}$. Since $\Omega^0_{C^c}$ is constant in the optimization problem (3.14), it can be ignored and we have that $\log|\Omega|$ and $\log|\Omega'|$ are equal up to a constant term. Furthermore, using again the fact that $\Omega \in \Theta_C(\Omega^0)$, we get

$$\begin{aligned} \operatorname{tr}[\Omega S] &= \operatorname{tr}[\Omega_C S_C] + \operatorname{tr}[\Omega_{C^c} S_{C^c}] + 2\operatorname{tr}[\Omega_{C,C^c} S_{C,C^c}] \doteq \operatorname{tr}[\Omega_C S_C] \\ &= \operatorname{tr}[\Omega' S_C] + \operatorname{tr}\left[\Omega^0_{C,C^c}(\Omega^0_{C^c})^{-1}\Omega^0_{C^c,C} S_C\right] \doteq \operatorname{tr}[\Omega' S_C]. \end{aligned}$$

Hence, the optimization problem (3.14) is equivalent to

$$\underset{\Omega' \in \mathcal{S}^{|C|}_{\succ 0}}{\text{maximize}} \quad \log|\Omega'| - \operatorname{tr}[S_C\Omega'].$$

Comparing this to the earlier discussions, this problem is equivalent to finding the maximum likelihood estimator of the precision matrix Ω' of the Gaussian graphical model associated to the graph $\mathcal{G}$ restricted to the nodes in C. Since C is a clique, the subgraph is complete and the maximum likelihood estimator is given by $\hat{\Omega}' = (S_C)^{-1}$. Hence, the solution to (3.14) is given by $\hat{\Omega} \in \Theta(\Omega^0)$ where

$$\begin{aligned} \hat{\Omega}_C &= \Omega' + \Omega^0_{C,C^c}(\Omega^0_{C^c})^{-1}\Omega^0_{C^c,C} \\ &= (S_C)^{-1} + \Omega^0_{C,C^c}(\Omega^0_{C^c})^{-1}\Omega^0_{C^c,C}. \end{aligned}$$

Hence, the solution to (3.14) is $\hat{\Omega} = T_C\Omega^0$. □

By Lemma 3.8, Algorithm 1 corresponds to an *iterative partial maximization* algorithm, or block coordinate descent algorithm. Since T_C is a linear transformation, it is continuous. Further, we showed that T_C maps $\mathcal{S}_{\succ 0}(\mathcal{G})$ onto itself. With these conditions satisfied, Lauritzen [21, Proposition A.3] proves that the iterative partial maximization algorithm converges, and hence Algorithm 1, to the maximum likelihood estimator $\hat{\Omega} \in \mathcal{S}_{\succ 0}(\mathcal{G})$.

3.3 Testing the subgraph hypothesis

In this Section, we apply the approximations developed in Section 2.6 to the problem of testing two nested Gaussian graphical models. More precisely, let $\mathcal{G} = (\Gamma, E)$ and $\mathcal{G}_0 = (\Gamma, E_0)$ with $E_0 \subset E$, we are interested in developing a test for the following hypothesis testing problem

$$H_0 : \Omega \in \mathcal{S}_{\succ 0}(\mathcal{G}_0) \quad \text{vs.} \quad H_1 : \Omega \in \mathcal{S}_{\succ 0}(\mathcal{G}) \setminus \mathcal{S}_{\succ 0}(\mathcal{G}_0). \tag{3.15}$$

The classical approach to this testing problem is to use the *likelihood ratio test* based on the *likelihood ratio statistic*. Given an observed covariance matrix S_n constructed from a sample of size n, the likelihood ratio statistic is given by

$$\Lambda(S_n) = -2 \left[\ell(\hat{\Omega}_{\mathcal{G}_0}(S_n)) - \ell(\hat{\Omega}_{\mathcal{G}}(S_n)) \right],$$

where $\hat{\Omega}_{\mathcal{G}_0}$ and $\hat{\Omega}_{\mathcal{G}}$ are the functions mapping an observed covariance matrix to the maximum likelihood estimators of the precision matrix under models $\mathcal{G}_0$ and $\mathcal{G}$ respectively. Under regularity conditions and assuming that the H_0 is true, the distribution of $\Lambda(S_n)$ converges to a χ^2_d distribution with $d = |E| - |E_0|$ degrees of freedom, see [28]. A hypothesis test in finite sample can then be constructed by using the χ^2_d approximation to the distribution of $\Lambda(S_n)$.

In Eriksen [16], the author gives the following simple example which demonstrates how the χ^2_d approximation fails when the sample size n is not large enough. Consider two graphs $\mathcal{G}$ and $\mathcal{G}_0$ with $p = 4$ nodes such that $\mathcal{G}_0$ is a cycle and $\mathcal{G}$ is a chordal cover of $\mathcal{G}_0$. We are interested in the hypothesis test displayed in Figure 7. Eriksen proposes an alternative test statistic for testing this class of problems which, in this example, is

$$Q(S_n) = \exp\left(-\Lambda(S_n)/n\right), \tag{3.16}$$

and demonstrates that it asymptotically follows a Beta distribution $B((n-3)/2, 1/2)$.

As we have seen in the previous section, the maximum likelihood estimator exists almost surely under both H_0 and H_1 if $n \geq 3$. We can empirically evaluate the χ^2_d approximation

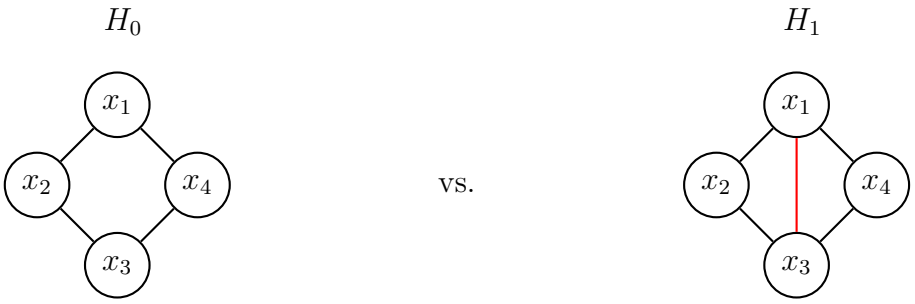


Figure 7: Simple hypothesis test proposed by Eriksen [16] for which the χ^2_1 distribution poorly approximated the distribution of the likelihood ratio statistic in small to medium sample sizes.

to the distribution of $\Lambda(S_n)$ and the $B((n-3)/2, 1/2)$ approximation to the distribution of $Q(S_n)$ by sampling the statistics under the null hypothesis of a chordless cycle. For a given sample size $n \in \mathbb{N}$, we sample $N = 10000$ values $\lambda_1, \dots, \lambda_N$ of the statistic $\Lambda(S_n)$ under the null hypothesis. With this sample, we construct the empirical cumulative distribution function $\hat{F}_\Lambda$ which approximates the true cumulative distribution function of $\Lambda(S_n)$, as well as the sorted empirical probabilities $\hat{p}_i = \hat{F}_\Lambda(\lambda_{(i)})$. Further, the empirical probabilities $\hat{p}_i$ can be compared to the probabilities $\tilde{p}_i = F(\lambda_{(i)})$ where F corresponds to the cumulative distribution function of either the χ^2_1 approximation of $\Lambda(S_n)$ or the $B((n-3)/2, 1/2)$ approximation of $Q(S_n) = \exp(-\Lambda(S_n)/n)$. Figure 8 displays this comparison. As seen in the upper pane of Figure 8, the χ^2_1 approximation is a poor approximation to the distribution of $\Lambda(S_n)$ while the $B((n-3)/2, 1/2)$ approximation to the distribution of $Q(S_n)$ is accurate even for small sample sizes. Since we are interested in constructing a hypothesis test based on these approximations, the small probability region is of particular interest. In the lower pane of Figure 8, we see that the χ^2_1 approximation is particularly poor for $n = 5$, where a test at level $\alpha = 0.05$ based on the χ^2_1 approximation would have a true size of 0.1.

While the $B((n-3)/2, 1/2)$ approximation seems accurate, its origin and accuracy are still unclear. The remainder of this section presents the construction of this statistic as well as proof of convergence. The following lemma from [16, Theorem 3.1] applies the p^* approximation to construct an accurate estimation to the density of the sufficient statistic S.

Lemma 3.9. Let $\mathcal{G}$ be a graph, let $\Omega \in \mathcal{S}_{\succ 0}(\mathcal{G})$ and let S_n be a sample covariance matrix computed from a sample $X = (X_1, \dots, X_n)$ of size $n \in \mathbb{N}$ of the Gaussian graphical model associated to $\mathcal{G}$ with precision matrix Ω. Then, the density $p(S; \Omega)$ of S satisfies the

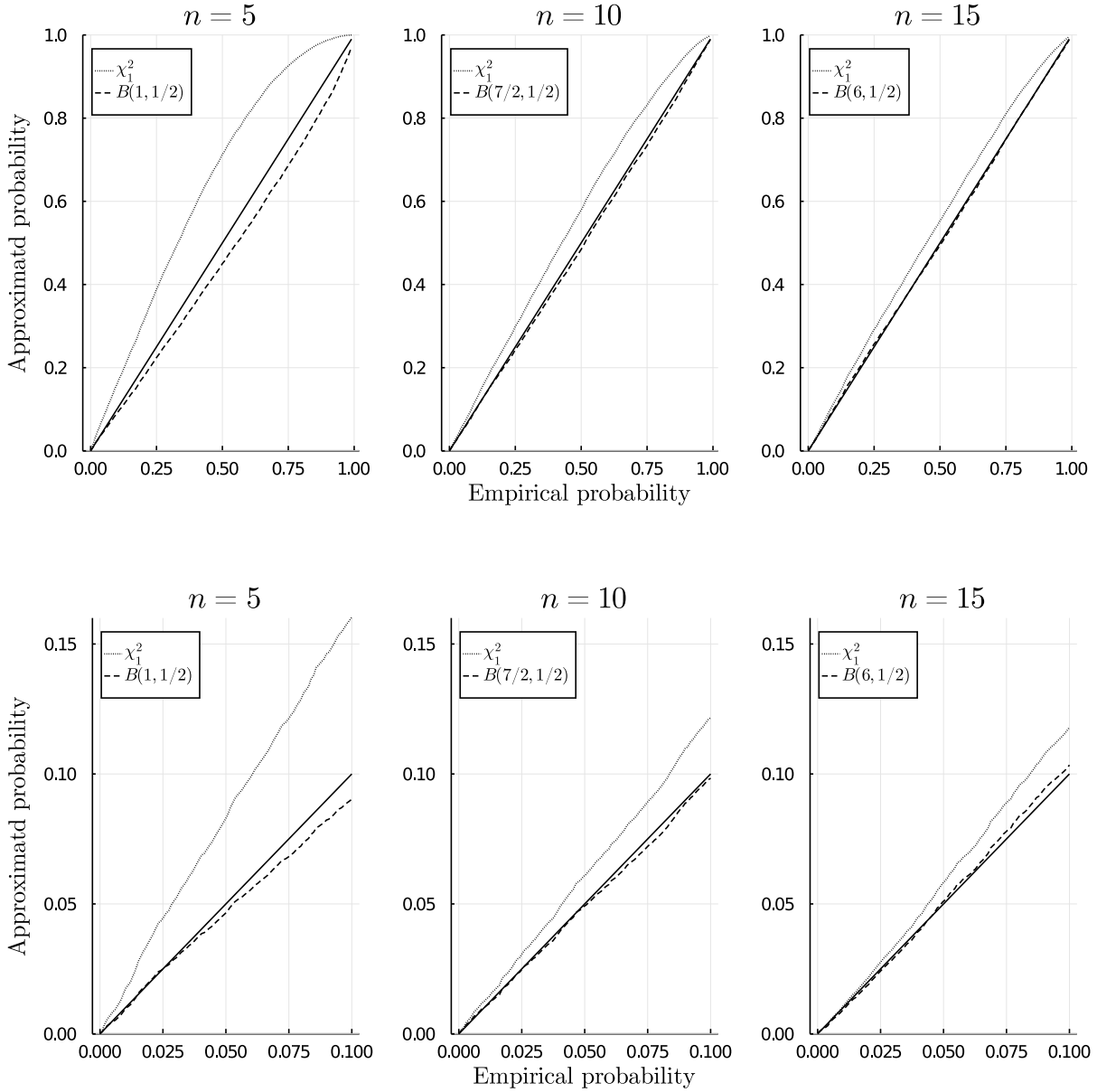


Figure 8: Comparison of the χ^2_1 approximation of the $\Lambda(S_n)$ statistic and Beta approximation of the $Q(S_n)$ statistic from Eriksen [16] for testing the null hypothesis of a chordless cycle given a sample of $n = 5, 10, 15$ observations. As seen in the upper pane, the χ^2_1 approximation poorly estimates the distribution of the $\Lambda(S_n)$ statistic for small and moderate sample sizes, while the $B((n-3)/2, 1/2)$ approximation to the distribution of $Q(S_n)$ is accurate even for small sample sizes. This is particularly strong when focusing on small probability regions as we show in the lower pane where the difference of probability can be of approximately 50%.

following,

$$p(S;\Omega) = c\frac{|\Omega|^{n/2}}{|\hat{\Omega}_{\mathcal{G}}(S)|^{n/2}}|j_{\mathcal{G}}(\hat{\Omega}_{\mathcal{G}}(S))|^{-1/2}\exp\left\{-\frac{n}{2}\text{tr}\left[\Omega S\right]\right\}(1+O(n^{-1})),$$

where c is a normalization constant, $\hat{\Omega}_{\mathcal{G}}(S)$ is the maximum likelihood of Ω assuming the graph $\mathcal{G}$ and given the data S, and j_G is the observed information matrix given by

$$j_{\mathcal{G}}(\Omega)_{ab} = \text{tr}\left[\Omega^{-1}H_a\Omega^{-1}H_b\right] \text{ for all } a,b \in E^*. \tag{3.17}$$

Proof. Since $XX^\top$ is sufficient in the Gaussian graphical model, S corresponds to the sample average of the sufficient statistic. Applying the p^* approximation to S as done in Section 2.6, it follows that the density of S satisfies

$$p(S;\Omega) = c|j_{\mathcal{G}}(\hat{\Omega}_{\mathcal{G}}(S))|^{-1/2}\exp\left\{\ell(\Omega;S) - \ell(\hat{\Omega}_{\mathcal{G}}(S);S)\right\}(1+O(n^{-1})).$$

Replacing the log-likelihood of the Gaussian graphical model in the above equation, we get that

$$\begin{aligned}
p(S;\Omega) &\propto |j_{\mathcal{G}}(\hat{\Omega}_{\mathcal{G}}(S))|^{-1/2}\exp\left\{\ell(\Omega;S) - \ell(\hat{\Omega}_{\mathcal{G}}(S);S)\right\}(1+O(n^{-1})) \\
&\propto |j_{\mathcal{G}}(\hat{\Omega}_{\mathcal{G}}(S))|^{-1/2}\frac{|\Omega|^{n/2}}{|\hat{\Omega}_{\mathcal{G}}(S)|^{n/2}}\exp\left\{-\frac{n}{2}\left(\text{tr}\left[\Omega S\right] - \text{tr}\left[\hat{\Omega}_{\mathcal{G}}(S)S\right]\right)\right\}(1+O(n^{-1})) \\
&\propto |j_{\mathcal{G}}(\hat{\Omega}_{\mathcal{G}}(S))|^{-1/2}\frac{|\Omega|^{n/2}}{|\hat{\Omega}_{\mathcal{G}}(S)|^{n/2}}\exp\left\{-\frac{n}{2}\text{tr}\left[\Omega S\right]\right\}(1+O(n^{-1}))
\end{aligned}$$

where the last statement follows from the fact that $\hat{\Omega}_{\mathcal{G}}(S)S = 1_p$ and hence $\text{tr}\left[\hat{\Omega}_{\mathcal{G}}(S)S\right] = p$ is constant. The formula for the observed infomation matrix can easily be verified by taking the appropriate derivatives of the log-likelihood. □

Before applying the result of Lemma 3.9 to the general problem of subgraph testing, we begin by studying a special case. Consider a Gaussian graphical model with graph $\mathcal{G} = ([p], E)$ and the sub-graph $\mathcal{G}_0$ constructed by removing a single edge $e_0 \in E$ from $\mathcal{G}$. The Gaussian graphical submodel is then associated to the subgraph $\mathcal{G}_0 = ([p], E_0)$ where $E_0 = E \setminus \{e_0\}$. Without loss of generality, we assume that $e_0 = \{1,2\}$. It follows that the

test statistic given in (3.16) is

$$\begin{aligned} Q(S_n) &= \exp\left(-\Lambda(S_n)/n\right) \\ &= \exp\left(2\left[\ell(\hat{\Omega}_{\mathcal{G}_0}(S_n)) - \ell(\hat{\Omega}_{\mathcal{G}}(S_n))\right]/n\right) \\ &= \exp\left((\log|\hat{\Omega}_{\mathcal{G}_0}(S_n)| - \operatorname{tr}[S_n\hat{\Omega}_{\mathcal{G}_0}(S_n)]) - (\log|\hat{\Omega}_{\mathcal{G}}(S_n)| - \operatorname{tr}[S_n\hat{\Omega}_{\mathcal{G}}(S_n)])\right) \\ &= \frac{|\hat{\Omega}_{\mathcal{G}_0}(S_n)|}{|\hat{\Omega}_{\mathcal{G}}(S_n)|}, \end{aligned}$$

where the last equality follows from the fact that $\operatorname{tr}[S_n\hat{\Omega}_{\mathcal{G}}(S_n)] = \operatorname{tr}[S_n\hat{\Omega}_{\mathcal{G}_0}(S_n)] = p$ is constant for any given graph $\mathcal{G}$. The following theorem from [16, Theorem 3.2], shows that the $Q(S_n)$ statistic asymptotically follows a Beta distribution with known parameters.

Theorem 3.10. Let $\mathcal{G} = ([p], E)$ be a graph with subgraph $\mathcal{G}_0 = ([p], E_0)$ satisfying $E \setminus E_0 = \{e_0\}$, where $e_0 = \{i, j\} \in E$. Let S be a sample covariance matrix computed from a sample of size $n > \operatorname{mlt}(\mathcal{G})$ of the Gaussian graphical model associated to $\mathcal{G}_0$ with precision matrix $\Omega_0 \in \mathcal{S}_{\succ 0}(\mathcal{G}_0)$. Then, the distribution of $Q(S_n)$ conditioned on observing S_n asymptotically converges to

$$B\left(\frac{n - f(e_0) - 1}{2}, \frac{1}{2}\right) \qquad \text{as } n \to \infty, \tag{3.18}$$

where $f(\{i, j\}) = |\operatorname{bd}(i) \cap \operatorname{bd}(j)|$.

Proof. We start by constructing approximations to the densities $p(S^{\mathcal{G}_0}; \Omega_0)$ and $p(S^{\mathcal{G}}; \Omega_0)$ by applying Lemma 3.9 in the Gaussian graphical models associated to $\mathcal{G}$ and $\mathcal{G}_0$ to get

$$p(S^{\mathcal{G}_0}; \Omega_0) = c\frac{|\Omega_0|^{n/2}}{|\hat{\Omega}_{\mathcal{G}_0}(S^{\mathcal{G}_0})|^{n/2}}|j_{\mathcal{G}_0}(\hat{\Omega}_{\mathcal{G}_0}(S^{\mathcal{G}_0}))|^{-1/2}\exp\left\{-\frac{n}{2}\operatorname{tr}\left[\Omega_0 S^{\mathcal{G}_0}\right]\right\}(1 + o(n^{-3/2}))$$

and

$$p(S^{\mathcal{G}}; \Omega_0) = c\frac{|\Omega_0|^{n/2}}{|\hat{\Omega}_{\mathcal{G}}(S^{\mathcal{G}})|^{n/2}}|j_{\mathcal{G}}(\hat{\Omega}_{\mathcal{G}}(S^{\mathcal{G}}))|^{-1/2}\exp\left\{-\frac{n}{2}\operatorname{tr}\left[\Omega_0 S^{\mathcal{G}}\right]\right\}(1 + o(n^{-3/2})).$$

Combining these results together allows us to approximate the density of S_e, conditioned

on $S^{\mathcal{G}_0}$, as follows

$$\begin{aligned} p(S_{e_0}|S^{\mathcal{G}_0};\Omega_0) &= \frac{p(S_{e_0},S^{\mathcal{G}_0};\Omega_0)}{p(S^{\mathcal{G}_0};\Omega_0)} = \frac{p(S^{\mathcal{G}};\Omega_0)}{p(S^{\mathcal{G}_0};\Omega_0)} \\ &\doteq \tilde{c}\frac{|\Omega_0|^{n/2}|\hat{\Omega}_{\mathcal{G}_0}(S^{\mathcal{G}_0})|^{-n/2}|j_{\mathcal{G}_0}(\hat{\Omega}_{\mathcal{G}_0}(S^{\mathcal{G}_0}))|^{-1/2}\exp\left\{-\frac{n}{2}\mathrm{tr}\left[\Omega_0 S^{\mathcal{G}_0}\right]\right\}}{|\Omega_0|^{n/2}|\hat{\Omega}_{\mathcal{G}}(S^{\mathcal{G}})|^{-n/2}|j_{\mathcal{G}}(\hat{\Omega}_{\mathcal{G}}(S^{\mathcal{G}}))|^{-1/2}\exp\left\{-\frac{n}{2}\mathrm{tr}\left[\Omega_0 S^{\mathcal{G}}\right]\right\}} \\ &= \tilde{c}\frac{|\hat{\Omega}_{\mathcal{G}}(S^{\mathcal{G}})|^{n/2}|j_{\mathcal{G}}(\hat{\Omega}_{\mathcal{G}}(S^{\mathcal{G}}))|^{1/2}}{|\hat{\Omega}_{\mathcal{G}_0}(S^{\mathcal{G}_0})|^{n/2}|j_{\mathcal{G}_0}(\hat{\Omega}_{\mathcal{G}_0}(S^{\mathcal{G}_0}))|^{1/2}} \\ &=: q^{n/2}\frac{|j_{\mathcal{G}}(\hat{\Omega}_{\mathcal{G}}(S^{\mathcal{G}}))|^{1/2}}{|j_{\mathcal{G}_0}(\hat{\Omega}_{\mathcal{G}_0}(S^{\mathcal{G}_0}))|^{1/2}}. \end{aligned}$$

where $q = |\hat{\Omega}_{\mathcal{G}}(S^{\mathcal{G}})|/|\hat{\Omega}_{\mathcal{G}_0}(S^{\mathcal{G}_0})|$. The last equality follows from the fact that $\Omega_0 S^{\mathcal{G}} = \Omega_0 S^{\mathcal{G}_0}$ which leads to the exponential terms canceling out. Since $q = \exp(-\Lambda(S)/n)$ and $\Lambda(S) \xrightarrow{d} \chi^2_1$ is asymptotically ancillary, q is also asymptotically ancillary. Further, since $S^{\mathcal{G}_0}$ is a complete sufficient statistic assuming $\mathcal{G}_0$, we have by Basu's Theorem [6] that $S^{\mathcal{G}_0}$ and q are asymptotically independent. Therefore it holds that, asymptotically, $p(S_{e_0};\Omega_0) = p(S_{e_0}|S^{\mathcal{G}_0};\Omega_0)$ for any $S^{\mathcal{G}_0}$ and we can chose $S^{\mathcal{G}_0}$ freely in the previous equation. By taking $S^{\mathcal{G}_0} = 1_p$, it follows that

$$S^{\mathcal{G}} = 1_p + S_{e_0}H_{e_0} = \begin{pmatrix} 1 & S_{e_0} & \\ S_{e_0} & 1 & \\ & & 1_{p-2} \end{pmatrix}.$$

Since $S^{\mathcal{G}_0}$ and $S^{\mathcal{G}}$ are positive definite, they are their own positive definite completion. Thus, we have $|\hat{\Omega}_{\mathcal{G}}(S^{\mathcal{G}})| = |S^{\mathcal{G}}|^{-1} = (1 - S^2_{e_0})^{-1}$ and $|\hat{\Omega}_{\mathcal{G}_0}(S^{\mathcal{G}_0})| = |S^{\mathcal{G}_0}|^{-1} = 1$, giving $q = 1 - S^2_{e_0}$. A change of variable from S_e to q has Jacobian $(1-q)^{-1/2}$ and the density of q is given by

$$p(q) \doteq \hat{c}q^{n/2}|j_{\mathcal{G}}(\hat{\Omega}_{\mathcal{G}}(S^{\mathcal{G}}))|^{-1/2}(1-q)^{-1/2}, \tag{3.19}$$

where $\hat{c}$ is a normalizing constant.

We now compute the determinant of the observed information matrix given in (3.17) with $\Omega^{-1} = 1_p + S_e H_e$. Let $a, b \in E^*$. we start by noting that for any $S \in \mathcal{S}(\mathcal{G})$ and $i, j \in [p]$

$$(SH_a)_{ij} = \begin{cases} S_{i\bar{j}} & \text{if } j \in a, \\ 0 & \text{otherwise} \end{cases} \quad \text{and} \quad (SH_b)_{ji} = \begin{cases} S_{j\bar{i}} & \text{if } i \in b, \\ 0 & \text{otherwise,} \end{cases}$$

where $\bar{j} \in a$ and $\bar{i} \in b$ are such that $\{j\} \cup \{\bar{j}\} = a$ and $\{i\} \cup \{\bar{i}\} = b$. By applying this in

the expression of $j_{\mathcal{G}}(S)_{ab}$, we get that

$$\operatorname{tr}[SH_aSH_b] = \sum_{i=1,j=1}^{p} (SH_a)_{ij}(SH_b)_{ji} = \sum_{(i,j)\in a\times b} S_{i\bar{j}}S_{j\bar{i}} = \sum_{e\in a\times b} S_eS_{\bar{e}}, \tag{3.20}$$

where the last equality follows by re-indexing and re-ordering the sum. Next, we inspect the different $a, b \in E^*$ and $e \in a \times b$ for which the summand $S_eS_{\bar{e}}$ is non-zero. Setting $s = S_{e_0}$, we have that $S = 1_p + sH_{e_0}$. Hence for any $e \in \{\{i, j\} : i, j \in [p]\}$

$$S_e = \begin{cases} 1 & \text{if } e = \{i\} \text{ for some } i \in [p], \\ s & \text{if } e = e_0, \\ 0 & \text{otherwise.} \end{cases}$$

Thus, the summands $S_eS_{\bar{e}}$ of (3.20) are non-zero if and only if both e and $\bar{e}$ are either $\{i\}$ for some $i \in [p]$ or equal to e_0. Without loss of generality, we assume that $e_0 = \{1, 2\}$. We can thus focus on the following cases.

Case 1. $e = \bar{e} = \{1, 2\}$. This is possible only if $a = \{1\}$ and $b = \{2\}$, in which case

$$j_{\mathcal{G}}(S)_{\{1\}\{2\}} = \sum_{e\in\{1\}\times\{2\}} S_eS_{\bar{e}} = S_{\{1,2\}}S_{\{1,2\}} = s^2.$$

Case 2. $e = \{1, 2\}$ and $\bar{e} = \{i, j\}$ with $i \neq j$ (or the opposite). Then, we must have $a = \{1, i\}$ and $b = \{2, j\}$ and since we assumed that $S = 1_p + sH_{e_0}$, we have that

$$j_{\mathcal{G}}(S)_{\{1,i\}\{2,j\}} = S_{12}S_{ij} + S_{1j}S_{i2} + S_{i2}S_{1j} + S_{ij}S_{12} = 0.$$

Case 3. $e = \{1, 2\}$ and $\bar{e} = \{i\}$ (or the opposite). This is the case when $a = \{1, i\}$ and $b = \{2, i\}$, and since $S_{ii} = 1$, $S_{12} = s$ and $S_{i1} = S_{i2} = 0$, we get

$$j_{\mathcal{G}}(S)_{\{1,i\}\{2,i\}} = S_{12}S_{ii} + S_{1i}S_{i2} + S_{i2}S_{1i} + S_{ii}S_{12} = 2s.$$

Note that the matrix $j_{\mathcal{G}}$ is indexed by edges in $\mathcal{G}$. Therefore, the cases $a = \{1, i\}$ and $b = \{2, i\}$ are only relevant if $a, b \in E$. In this case, i is a neighbour of both 1 and 2, meaning that $i \in \operatorname{bd}(1) \cap \operatorname{bd}(2) =: C$.

Case 4. $e = \{i\}$ and $\bar{e} = \{j\}$. This only happens if $a = b = \{i, j\}$, which, again using

that $a, b \in E$ and $S = 1_p + sH_{e_0}$, gives

$$j_{\mathcal{G}}(S)_{\{i,j\}\{i,j\}} = \begin{cases} S_{ii}S_{ii} = 1 & \text{if } i = j, \\ 2S_{11}S_{22} + 2S_{12}S_{12} = 2 + 2s^2 & \text{if } \{i,j\} = \{1,2\}, \\ 2S_{ii} + 2S_{ij} = 2 & \text{otherwise.} \end{cases}$$

This shows that $j_{\mathcal{G}}(S)$ is a block diagonal matrix with blocks each equal to one of the following matrices,

$$A = \begin{array}{c} \\ \{1\} \\ \{2\} \\ \{1,2\} \end{array} \begin{array}{c} \begin{array}{ccc} \{1\} & \{2\} & \{1,2\} \end{array} \\ \begin{pmatrix} 1 & s^2 & 2s \\ s^2 & 1 & 2s \\ 2s & 2s & 2+2s^2 \end{pmatrix} \end{array} \qquad B_i = \begin{array}{c} \\ \{1,i\} \\ \{2,i\} \end{array} \begin{array}{c} \begin{array}{cc} \{1,i\} & \{2,i\} \end{array} \\ \begin{pmatrix} 2 & 2s \\ 2s & 2 \end{pmatrix} \end{array}, \text{ for } i \in C.$$

Since $|A| = 2(1-s^2)^3$ and $|B_i| = 4(1-s^2)$ for $i \in C$, we have that the determinant of the observed information $|j_{\mathcal{G}}(1_p + sH_{e_0})| \propto (1-s^2)^{3+|C|}$ is equal to $(1 - S_{e_0}^2)^{3+f(e_0)} = q^{3+f(e_0)}$. Replacing this equality in (3.19) gives us,

$$\begin{aligned} p(q) &\doteq \hat{c} q^{n/2} |j_{\mathcal{G}}(\hat{\Omega}_{\mathcal{G}}(S^{\mathcal{G}}))|^{-1/2} (1-q)^{-1/2} \\ &\propto q^{n/2} q^{-(3+f(e_0))/2} (1-q)^{-1/2} \\ &= q^{(n-f(e_0)-3)/2} (1-q)^{-1/2}. \end{aligned}$$

Since the density of a $B(\alpha, \beta)$ distribution is proportional to $q^{\alpha-1}(1-q)^{\beta-1}$, we have that q asymptotically follows a $B((n - f(e_0) - 1)/2, 1/2)$ distribution. □

This construction can be generalized to the case where $\mathcal{G}_0 = ([p], E_0)$ is the subgraph of $\mathcal{G} = ([p], E)$ with $d = |E \setminus E_0| > 1$. Let $E_- = E \setminus E_0 = \{e_0, \ldots, e_{d-1}\}$. We define for $i = 1, \ldots, d-1$ the subgraphs $\mathcal{G}_i = ([p], E_i)$ with $E_i = E_{i-1} \cup \{e_i\}$. Then, the $Q(S_n)$ statistic can be decomposed as follows,

$$\begin{aligned} Q(S_n) &= \frac{|\hat{\Omega}_{\mathcal{G}_0}(S_n)|}{|\hat{\Omega}_{\mathcal{G}}(S_n)|} = \frac{|\hat{\Omega}_{\mathcal{G}_0}(S_n)|}{|\hat{\Omega}_{\mathcal{G}_{d-1}}(S_n)|} \\ &= \frac{|\hat{\Omega}_{\mathcal{G}_0}(S_n)|}{|\hat{\Omega}_{\mathcal{G}_1}(S_n)|} \frac{|\hat{\Omega}_{\mathcal{G}_1}(S_n)|}{|\hat{\Omega}_{\mathcal{G}_2}(S_n)|} \cdots \frac{|\hat{\Omega}_{\mathcal{G}_{d-2}}(S_n)|}{|\hat{\Omega}_{\mathcal{G}_{d-1}}(S_n)|} =: Q_{0,1}(S_n) Q_{1,2}(S_n) \ldots Q_{d-2,d-1}(S_n), \end{aligned}$$

where $Q_{i,i+1}(S_n) = |\hat{\Omega}_{\mathcal{G}_i}(S_n)| / |\hat{\Omega}_{\mathcal{G}_{i+1}}(S_n)|$ corresponds to the test statistic for testing the

submodel $\mathcal{G}_i$ in $\mathcal{G}_{i+1}$. Applying Theorem 3.10 to each $Q_{i,i+1}(S_n)$ gives that, asymptotically,

$$Q_{i,i+1}(S_n) \sim B\left(\frac{n - f(e_i) - 1}{2}, \frac{1}{2}\right) =: B(\alpha_i, 1/2),$$

where for $e_i = \{j, k\}$, $f(e_i) = |\mathrm{bd}(j) \cap \mathrm{bd}(k)|$ is evaluated in the graph $\mathcal{G}_{i+1}$. Hence, $Q(S_n)$ is asymptotically distributed as the product of independent $B(\alpha_i, 1/2)$ random variables. We call the approximation to the distribution of $Q(S_n)$ resulting from this procedure the Eriksen approximation and the resulting statistical test the Eriksen test.

3.4 Simulation studies

We now compare different properties of the likelihood ratio test and Eriksen test described in Section 3.3. We are interested in evaluating the size and power of the tests resulting from these two asymptotic approximations. The *size* of a test is its probability of rejecting the null hypothesis when it is true, also called *type I error*. The *power* of a test is its probability to reject the null hypothesis when it is false. One is interested in tests maximizing power while keeping the probability of doing a type I error under a pre-defined level α. In other words, a good test maximizes the probability of discovering true phenomena while maintaining a low probability of making a false discovery.

We now present experiments aiming at exploring the size and power of the statistical tests constructed based on the χ^2_d approximation to the distribution of the $\Lambda(S_n)$ statistic and the product of Betas approximation to the distribution of the $Q(S_n)$ statistic. In particular, we are interested in evaluating how the different tests behave when the sample size is kept fix and the number of parameters increases.

Note that the Eriksen approximation to the distribution of $Q(S_n)$ is based on the product of independent Beta distributed random variables $\prod_{i=1}^d B_i$, which does not admit a closed form. Instead, we construct an estimator to the distribution of $\prod_{i=1}^d B_i$ by sampling 100 000 observations of the vector $(B_1, \ldots, B_d)$ and use the product of the sample to construct the empirical estimator to the distribution function.

In the first setup, we consider a sequence of problems in which the number of nodes in a graph $\mathcal{G}$ grows while the number of edges removed to form $\mathcal{G}_0$ is kept fix. In particular, we consider the complete graph $\mathcal{G} = ([p], E)$ with $E = \{\{i, j\} : i, j \in [p], i \neq j\}$ and the subgraph $\mathcal{G}_0 = ([p], E_0)$ with $E_0 = E \setminus \{\{1, 3\}, \{2, 4\}\}$. As shown in Figure 9, the subgraph $\mathcal{G}_0$ can be decomposed into the cycle $\{1, 2, 3, 4\}$ and the clique $C_p = [p] \setminus \{1, 2, 3, 4\}$ formed with the rest of the nodes, such that each node of the cycle forms a clique when added to C.

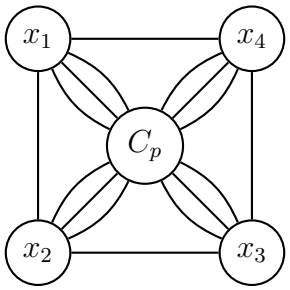


Figure 9: The graph $\mathcal{G}_0$ depicted here is a subgraph of the complete graph $\mathcal{G}$ which encodes a constant number of independence constraints as p grows.

In this setup, the quantities of interest are the entries of the precision matrix corresponding to the two edges removed from $\mathcal{G}$ to construct $\mathcal{G}_0$, Ω_{13} and Ω_{24}. We call *nuisance parameters* the other entries of Ω which are not tested in the model comparison. Hence, in this setup, while the number of parameters of interest corresponding to the constraints encoded in $\mathcal{G}_0$ is fix, the number of nuisance parameters grows quadratically with p. In this hypothesis test, $d = |E| - |E_0| = 2$ and hence the likelihood ratio statistic $\Lambda(S_n)$ asymptotically follows a χ^2_2 distribution. Following the procedure described in Section 3.3, the $Q(S_n)$ statistic is asymptotically distributed as the product of two independent Beta distributed random variables $B((n - f(\{1,3\}) - 1), 1/2)$ and $B((n - f(\{2,4\}) - 1), 1/2)$. Regardless of the order in which the edges are removed, we have that $f(\{2,4\}) = f(\{1,3\}) = p - 2$. Thus $Q(S_n)$ is asymptotically distributed as $B((n-p+1)/2, 1/2)B((n-p+1)/2, 1/2)$.

To evaluate the size of each approximation, we follow the numerical procedure used in Tang et al. [27]. For a fixed sample size $n = 100$ and values $p = 5, 10, 20, 50, 75, 90$, we perform a series of experiments with the goal of evaluating the approximations of the respective test statistics under the null hypothesis. In each experiment, we execute the following procedure

1. Sample a random precision matrix $\Omega \in \mathcal{S}(\mathcal{G}_0)$ as described in Appendix A.
2. Sample a set of observations $X_1, \ldots, X_n \overset{iid}{\sim} N_p(0, \Omega^{-1})$ and compute the sufficient statistic $S_n = XX^\top/n$.
3. Compute the test statistics $\Lambda(S_n)$ and $Q(S_n)$.
4. Compute p-values based on the asymptotic approximations to the distribution of the test statistics.

Repeating the experiment $N = 25\,000$ times provides a large sample of p-values for each constructed test. Under the null hypothesis, the approximate distributions are asymptotically valid, hence the p-values are asymptotically uniform on $[0, 1]$. As shown in the

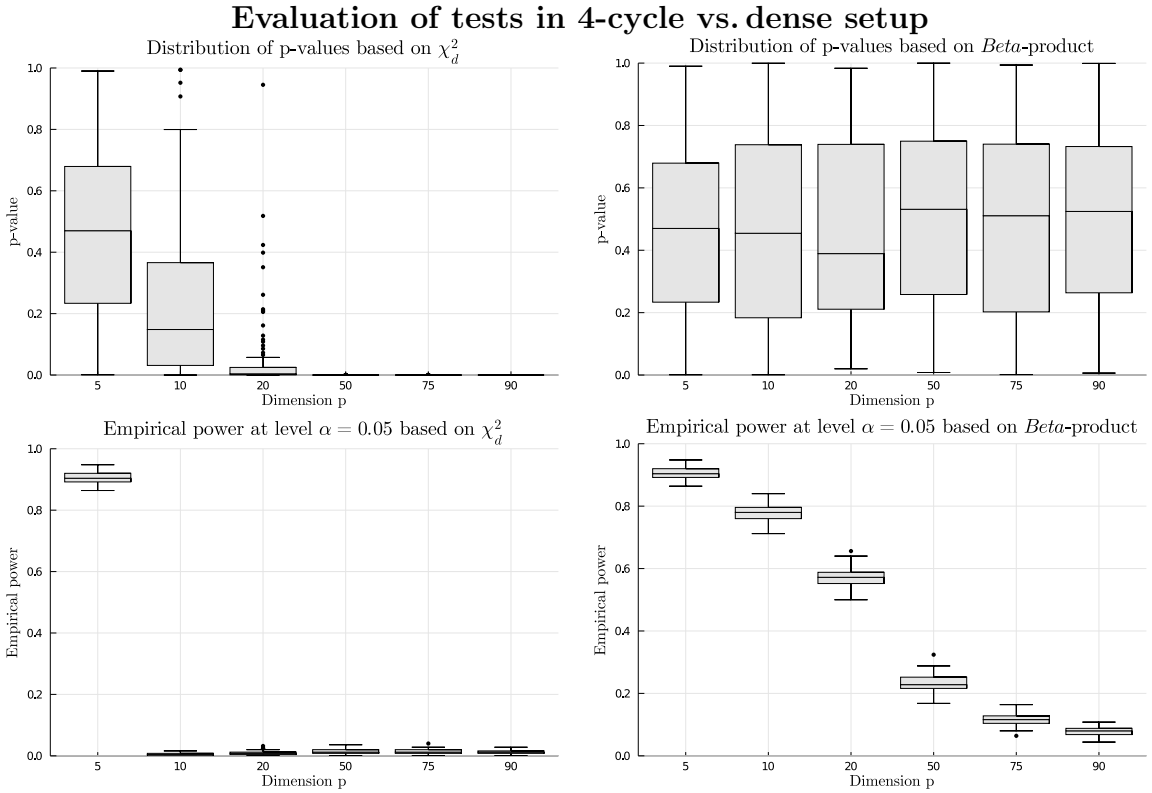


Figure 10: Evaluation of the tests based on the χ^2_d and Eriksen approximations for $n = 100$ and $p = 5, 10, 20, 50, 75, 90$. The null hypothesis corresponds to the complete graph minus two edges, forming a 4-cycle and the alternative hypothesis is the complete graph. The upper panes show the distribution of p-values when the data is sampled from the null hypothesis. The lower pane displays the Monte-Carlo estimate of the rejection rate of each test when the data is sampled from the alternative hypothesis.

upper pane of Figure 10, the distribution of the p-values in the likelihood ratio test is not uniform for $p \geq 10$. On the other hand, the p-values for the Eriksen test appear to remain uniform even for p approaching n.

To evaluate the power of each test, we estimate the empirical rejection rate under the alternative hypothesis given a fix nominal level $\alpha = 0.05$. Similarly to the evaluation of the size of each test, we fix the sample size $n = 100$ and perform experiments for different values of $p = 5, 10, 20, 50, 75, 90$. For estimating the power of a test, we adapt step 1 of the experiment described above with sampling Ω from the alternative hypothesis instead of the null hypotheses to have $\Omega \in \mathcal{S}_{\succ 0}(\mathcal{G}) \setminus \mathcal{S}_{\succ 0}(\mathcal{G}_0)$. With a sample of $N = 25\ 000$ p-values from each test, we compute the Monte-Carlo estimate of the average test power at level $\alpha = 0.05$ by dividing the number of p-values falling under this threshold by N. We visualize these results in the lower pane of Figure 10, in which we can see that both tests suffer from a strong loss of power as the number of nodes in the graph grows.

Algorithm 2 Compute Betas for approximation of $Q(S_n)$ in p-cycle vs. complete problem

Input: Number of nodes p.
Output: Parametrized beta variables for approximating the distribution of $Q(S_n)$.

```
Let Betas= {}
Let G = ([p], E) be the complete graph over [p]
for i = 1, ..., p − 2 do
    for j = i + 2, ..., p do
        if {i, j} = {1, p} then
            Skip iteration
        end if
        Set E := E \ {{i, j}} and G := ([p], E)
        Let C = |bd_G(i) ∩ bd_G(j)|
        Set Betas = Betas ∪ {B((n − C − 1)/2, 1/2)}
    end for
end for
Return Betas
```

Next, we consider a second setup, in which the number of edges removed from $\mathcal{G}$ to form $\mathcal{G}_0$ grows with the number of nodes in $\mathcal{G}$. We define $\mathcal{G}$ to be a complete graph over p nodes and $\mathcal{G}_0$ to be the p-cycle defined in Example 3.6. In this case, we have p nuisance parameters corresponding to the edges in $\mathcal{G}_0$ and we have $p(p-1)/2$ parameters of interest corresponding to the edges removed from $\mathcal{G}$. Further, in this setup, $d = |E| - |E_0| = p(p-1)/2 - p = p(p-3)/2$. Hence, $\Lambda(S_n)$ is asymptotically $\chi^2_{p(p-3)/2}$. The Eriksen approximation to the distribution of $Q(S_n)$ is a product of $p(p-3)/2$ random variables following Beta distributions. To compute the parameters of these Beta distributions, we iteratively remove edges from $\mathcal{G}$ following a lexicographical ordering: $\{1,3\}, \{1,4\}, \ldots, \{1,p-1\}, \{2,4\}, \ldots, \{2,p\}, \{3,5\} \ldots, \{p-2,p\}$. For each edge removed, the graph is updated and the parameters of the corresponding Beta random variable are computed. The detailed algorithm is displayed in Algorithm 2.

We evaluate the size of each test following the same procedure as in the previous setup. The result displayed in the upper pane of Figure 11 shows that the χ^2_d approximation only properly approximates the distribution of $\Lambda(S_n)$ under the null hypothesis when the dimension p is kept low. This time however, the Eriksen approximation is only accurate for $p \leq 20$.

Similarly for the power, we use the same procedure as in the previous setup with the same nominal level $\alpha = 0.05$. While the lower pane of Figure 11 shows that the χ^2_d approximation suffers from the same loss of power for $p > 10$, the test based on the $Q(S_n)$ statistic has a power of 1 in every setup. This could be explained by the large difference between the null and alternative hypotheses.

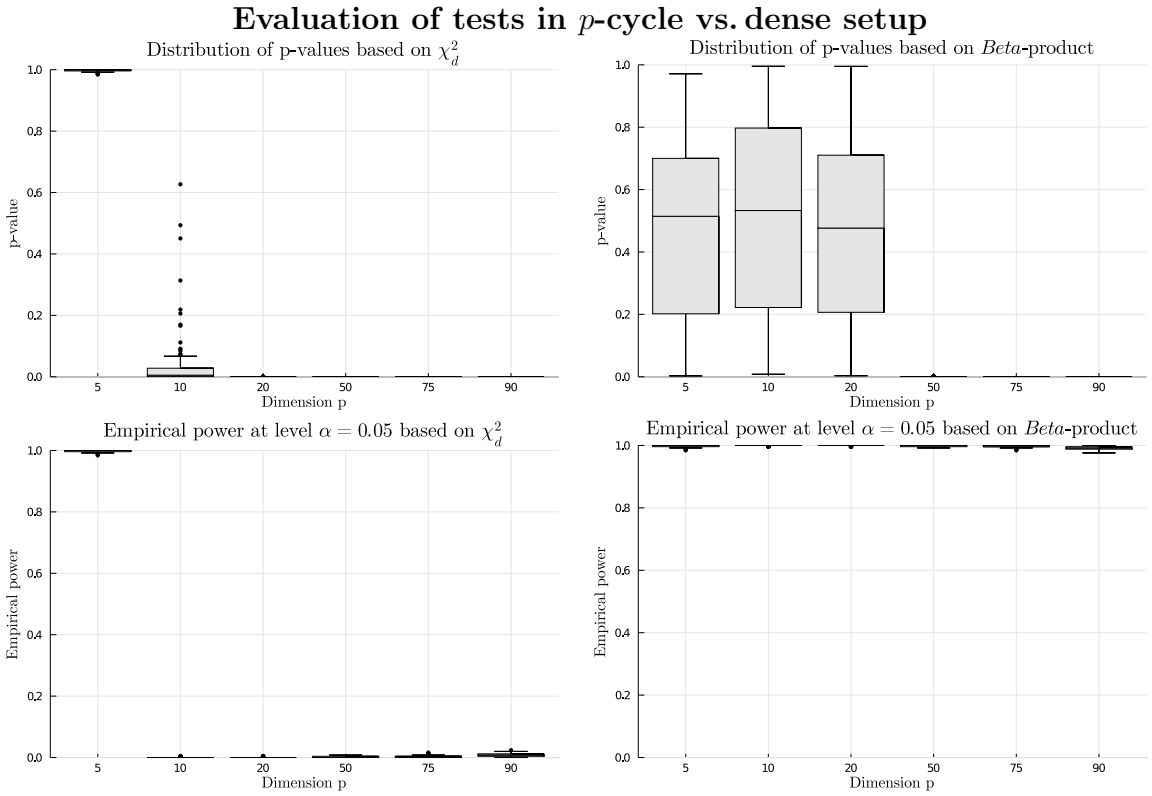


Figure 11: Evaluation of the tests based on the χ^2_d and Eriksen approximations for $n = 100$ and $p = 5, 10, 20, 50, 75, 90$. The upper panes show the distribution of p-values when the data is sampled from the null hypothesis. The null hypothesis corresponds to a p-cycle and the alternative hypothesis is the complete graph. The lower pane displays the Monte-Carlo estimate of the rejection rate of each test when the data is sampled from the alternative hypothesis.

4 Conclusion

This thesis studied an alternative statistical test to the likelihood ratio test for testing two alternative nested Gaussian graphical models. The test introduced by Eriksen [16] involves exploiting the graph structure of the nested models to adapt general results from higher-order statistic.

We presented an introduction and analysis of the tools from higher-order statistics required to develop the new statistical test, resulting in the p^* approximation to the distribution of the maximum likelihood estimator. We then studied the maximum likelihood problem in Gaussian graphical models and the conditions under which a solution exists. By studying both the primal and dual form of the likelihood maximization problem, we were able to link this problem to a matrix completion problem. This allowed us to exploit existence results from matrix completion theory in the context of likelihood maximization. Further, we derived the test presented in Eriksen [16] as a special case of the p^* approximation in Gaussian graphical models.

A collection of simulations helped us understand the size and power of the Eriksen test and compare it to the likelihood ratio test. By studying different graph topologies and by varying the dimensionality of the problem, we were able to numerically show that the Eriksen test, unlike the likelihood ratio test, is robust to an increase in the number of nuisance parameters. Furthermore, the Eriksen test was favorable both in terms of size and power, even with increasing the number of parameters of interest, compared to the likelihood ratio test.

Results in higher-order statistics explain why the Eriksen test favorably compared to the likelihood ratio test in terms of size. However, these results do not cover the behaviour of the test under the null hypothesis. This leaves the opportunity to develop an understanding of the benefits of the Eriksen test in terms of power. Furthermore, all proofs presented in this thesis only cover asymptotic theory, in which the dimensionality of the problem is fix. It would be interesting to better understand why the test based on the p^* approximation appears to be both robust to an increase of the number of nuisance parameters, and less sensitive than the likelihood ratio test to an increase of the number of parameters of interest.

A Sampling of random precision matrices

In this Appendix, we discuss the method employed to generate a random precision matrix $\Omega \in \mathcal{S}_{\succ 0}(\mathcal{G})$ given some graph $\mathcal{G} = ([p], E)$. We begin with the assumption that $\mathcal{G}$ is complete. In this case, generating $\Omega \in \mathcal{S}_{\succ 0}(\mathcal{G})$ is equivalent to sampling a random element of $\mathcal{S}^p_{\succ 0}$.

Suppose $X_1, \ldots, X_n \overset{iid}{\sim} N(0, 1_p)$ with $n > p$ and let $X = (X_1, \ldots, X_n) \in \mathbb{R}^{p \times n}$. Then the $p \times p$ matrix $\Omega = XX^\top$ is almost surely invertible and is positive definite. This construction defines a distribution over the space of $p \times p$ positive definite matrices called the *Wishart distribution* writen $\mathcal{W}(1_p, n)$. We can sample from the Wishart distribution by following the construction described before, or, more efficiently via the *Bartlett decomposition* [25] of Ω. Let L be a lower triangular matrix with independent random entries given by

$$L_{ij} \sim \begin{cases} N(0,1) & \text{if } i > j, \\ \chi^2_{p-i+1} & \text{if } i = j. \end{cases}$$

The matrix $\Omega = LL^\top$ then follows a Wishart distribution $\mathcal{W}(1_p, n)$. This sampling scheme requires sampling less scalar random variables and provides, by construction, the Cholesky decomposition of Ω, which makes numerical manipulations of Ω more efficient and stable.

Let us now consider the case when $\mathcal{G} = ([p], E)$ is constructed by taking the complete graph over the nodes $[p]$ and removing the edge $e = \{i, j\}$ for $i, j \in [p]$. In this case, sampling a random matrix $\Omega \in \mathcal{S}_{\succ 0}(\mathcal{G})$ is equivalent to sampling a matrix in the subspace $\mathcal{S}^p_{\succ 0} \cap \{\Omega_e = 0\}$. One approach would be to sample $\Omega \sim \mathcal{W}(1_p, n)$ for $n > p$ and set $\Omega_e = 0$. However, the resulting matrix might not be positive definite which makes this sampling scheme unsuited.

Let L be sampled as described above and let $\Omega = LL^\top$. Then, if L has rows L_i, we have that $\Omega_e = \Omega_{ij} = L_a L_b^\top$ and hence

$$\Omega_e = 0 \Leftrightarrow L_i \perp L_j.$$

Therefore, we can remove the edge e from Ω by orthogonalizing the corresponding columns in L before constructing Ω. To do this, we define the matrix L^e via a transformation the rows L_i of L

$$L^e_k = \begin{cases} L_i - \frac{L_i L_j^\top}{L_j L_j^\top} L_j & \text{if } k = i, \\ L_k & \text{otherwise.} \end{cases}$$

Since this step involves subtracting one row from another in the matrix L, we have that

$|L^e| = |L|$. Hence, the matrix $\Omega^e = L^e(L^e)^\top$ is positive definite and satisfies $\Omega^e_e = 0$. This edge removal corresponds to a single step in the Gram-Schmidt orthogonalization process. Hence, if more than one edge have to be removed, a complete Gram-Schmidt algorithm can be run on the rows of L as described in Algorithm 2 of Córdoba et al. [11].

References

[1] Discussion on Dr. Cox's Paper. *Journal of the Royal Statistical Society: Series B (Methodological)*, 20(2):232–242, 1958.

[2] O.E. Barndorff-Nielsen. Conditionality resolutions. *Biometrika*, 67(2):293–310, 1980.

[3] O.E. Barndorff-Nielsen. On a formula for the distribution of the maximum likelihood estimator. *Biometrika*, 70(2):343–365, 1983.

[4] O.E. Barndorff-Nielsen, D.R. Cox, and H.F.D.R. Cox. *Asymptotic Techniques for Use in Statistics*. Asymptotic Techniques for Use in Statistics. Springer US, 1989.

[5] Maurice Stevenson Bartlett. Properties of sufficiency and statistical tests. *Proceedings of the Royal Society of London. Series A-Mathematical and Physical Sciences*, 160(901):268–282, 1937.

[6] D. Basu. On statistics independent of a complete sufficient statistic. *Sankhyā: The Indian Journal of Statistics (1933-1960)*, 15(4):377–380, 1955.

[7] Luis Benet and David P. Sanders. A Julia package for Taylor expansions in one or more independent variables. `https://github.com/JuliaDiff/TaylorSeries.jl`.

[8] Jeff Bezanson, Alan Edelman, Stefan Karpinski, and Viral B Shah. Julia: A fresh approach to numerical computing. *SIAM review*, 59(1):65–98, 2017.

[9] Stephen Boyd, Stephen P Boyd, and Lieven Vandenberghe. *Convex optimization*. Cambridge university press, 2004.

[10] Søren Ladegaard Buhl. On the existence of maximum likelihood estimators for graphical gaussian models. *Scandinavian Journal of Statistics*, 20:263–270, 1993.

[11] Irene Córdoba, Gherardo Varando, Concha Bielza, and Pedro Larrañaga. On generating random gaussian graphical models. *International Journal of Approximate Reasoning*, 125:240–250, 2020.

[12] David Roxbee Cox and Ole E Barndorff-Nielsen. *Inference and asymptotics*, volume 52. CRC Press, 1994.

[13] Henry E Daniels. Saddlepoint approximations in statistics. *The Annals of Mathematical Statistics*, pages 631–650, 1954.

[14] A. P. Dempster. Covariance selection. *Biometrics*, 28(1):157–175, 1972.

[15] Rick Durrett. *Probability: Theory and Examples*. Cambridge Series in Statistical and Probabilistic Mathematics. Cambridge University Press, 5 edition, 2019.

[16] P Svante Eriksen. Tests in covariance selection models. *Scandinavian journal of statistics*, pages 275–284, 1996.

[17] Robert Grone, Charles R. Johnson, Eduardo M. Sá, and Henry Wolkowicz. Positive definite completions of partial hermitian matrices. *Linear Algebra and its Applications*, 58:109–124, 1984.

[18] Elizabeth Gross and Seth Sullivant. The maximum likelihood threshold of a graph. *Bernoulli*, 24(1):386 – 407, 2018.

[19] Ernst Ising. Beitrag zur theorie des ferromagnetismus. *Zeitschrift für Physik*, 31(1):253–258, 1925.

[20] John E Kolassa. *Series approximation methods in statistics*, volume 88. Springer Science & Business Media, 2006.

[21] Steffen L. Lauritzen. *Graphical Models*. Oxford University Press, 1996.

[22] Erich L Lehmann and George Casella. *Theory of point estimation*. Springer Science & Business Media, 2006.

[23] Marloes Maathuis, Mathias Drton, Steffen Lauritzen, and Martin Wainwright. *Handbook of graphical models*. CRC Press, 2018.

[24] Aaron Meurer, Christopher P. Smith, Mateusz Paprocki, Ondřej Čertík, Sergey B. Kirpichev, Matthew Rocklin, AMiT Kumar, Sergiu Ivanov, Jason K. Moore, Sartaj Singh, Thilina Rathnayake, Sean Vig, Brian E. Granger, Richard P. Muller, Francesco Bonazzi, Harsh Gupta, Shivam Vats, Fredrik Johansson, Fabian Pedregosa, Matthew J. Curry, Andy R. Terrel, Štěpán Roučka, Ashutosh Saboo, Isuru Fernando, Sumith Kulal, Robert Cimrman, and Anthony Scopatz. Sympy: symbolic computing in python. *PeerJ Computer Science*, 3:e103, January 2017.

[25] W. B. Smith and R. R. Hocking. Algorithm as 53: Wishart variate generator. *Journal of the Royal Statistical Society. Series C (Applied Statistics)*, 21(3):341–345, 1972.

[26] Terence P Speed and Harri T Kiiveri. Gaussian markov distributions over finite graphs. *The Annals of Statistics*, pages 138–150, 1986.

[27] Y. Tang and N. Reid. Modified likelihood root in high dimensions. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, August 2020.

[28] Samuel S Wilks. The large-sample distribution of the likelihood ratio for testing composite hypotheses. *The annals of mathematical statistics*, 9(1):60–62, 1938.