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.

Munich,

Acknowledgements

Abstract

Zusammenfassung

Contents

Contents **1**

1 Introduction **2**

2 Higher-order statistics **4**
2.1 The characteristic function and related quantities 4
2.2 A heuristic introduction to the Edgeworth expansion 11
2.3 Convergence of the Edgeworth expansion 15
2.4 A numerical case study of the Edgeworth approximation 20
2.5 Saddlepoint approximation 22
2.6 The p^* approximation in exponential families 27
2.7 Julia implementation of higher-order approximations 33

3 Gaussian Graphical Models **37**
3.1 Preliminaries 37
3.2 MLE in Gaussian graphical models 38
3.3 Hypothesis testing 49

References **55**

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 interaction networks and the way the biological expression of genes interact with each other to better understand the development of diseases. In statistical mechanics, the Ising model [18] 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 the $\mathcal{G}$ represent entries of the random vector, and missing edges represent conditional independence constraints between 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 will 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 be studied under the name of *covariance selection models* as introduced by Dempster [13].

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 $\mathcal{P}_0 = \{P_\theta : \theta \in \Theta_0\}$ 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 problem is the likelihood ratio test. The likelihood ratio test provides a generic approach based on the difference in maximum likelihood attainable in each model that can be applied in a wide variety of model. Assuming the null hypothesis 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 result might not work well in finite sample and could be vastly improved by considering corrected versions of the likelihood ratio statistics. In a influential paper, Bartlett [5] shows that the likelihood ratio could be adjusted with a multiplicative factor to improve the accuracy of the χ^2 approximation. Later, similar methods exploiting higher-order expansions of the characteristic function were developed under the term of *higher-order statistics* to construct asymptotic approximation and statistic adjustments with high-accuracy in a small samples. Barndorff-Nielsen and Cox [4, 11] offers a wide overview of the development and application of such methods.

In this thesis, we are intersted in studying uses of higher-order approximations for testing subgraph null hypotheses of Gaussian graphical models. Eriksen [15] shows that the χ^2 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. In this thesis, we present the work of Eriksen and empirically show that it can also 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 converge proofs based on the modern presentation of Kolassa [19]. In Chapter 3, we bring our attention to Gaussian graphical models and present selected results concerning the existence of maximum likelihood estimator. We then apply higher-order methods to submodel selection in Gaussian graphial models following the work of Eriksen [15]. 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.

2 Higher-order statistics

This chapter introduces the necessary theoretical tools to construct and study higher-order statistics. In Section (ref), we first give a review of the role and properties of the characteristic function to study continuous multivariate distributions. In Section (ref), we show how the results presented before can used to construct the Edgeworth series approximation to the density of a standardized sum. We then study the convergence of this approximation scheme and illustrate theoretical results by applying it to simple distributions. In Section (ref), we present the Saddlepoint approximation. We compare it to the Edgeworth approximation and demonstrate how it can be used to approximate the density of the maximum likelihood estimator in an exponential family, linking Saddlepoint approximations to the p^* approximation. Finally, 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* in a central tool in studying probability distributions. In this first section, we review general results about the characteristic function of a multivariate continuous distribution. 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 theorem shows that under regularity conditions on the characteristic function, the density of a random vector can be shown to exist and 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 [14], 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 since 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 $\mathbb{R}^p$. Furthermore, using the same absolute convergence property and by Fubini's Theorem the order of integration can be changed, yielding

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

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 Fourier transforms will allow us to study approximations of densities constructed that are not necessarily themselves densities and characteristic functions. We will use a definition of the Fourier transform slightly different from the common one, in which the sign of the exponent is reversed. For $f \in L^1(\mathbb{R}^p)$, the Fourier transform $\mathcal{F}[f]$ 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 can generalize Theorem 2.1 to provide the necessary conditions under which the Fourier transform can be inverted.

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 it's positive and negative part 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 characteristic functions ζ^+ and ζ^-. We can replace these quantities in (2.3) to have

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

By applying Theorem 2.1 to the positive and negative parts of f, we obtain that

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

and 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 theorem lets us extend the notation introduced in Equation (2.2) and define the inverse Fourier transform operator $\mathcal{F}^{-1}$ as in Equation (2.4),

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

Better understanding the characteristic function also requires to better understand in which space of function it lies. In this lemma, we relate L^p integrability of the characteristic function to the existence of the density of a convolution of random variables.

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

Proof. This proof is an adaptation of the one-dimensional proof given in [19, Lemma 2.4.4].

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

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

and hence $\xi^l \in L^1(\mathbb{R}^p)$. Since ξ^l is the characteristic function of a sum of l independent copies of X, Theorem 2.1 applies and the density of the convolution of l copies of X exists and is bounded.
We now prove the *if* direction of the theorem. Assume that there exists a $j \in \mathbb{N}$ such that the density f_j of a convolution of j independent copies of X exists and is bounded. Then, for any $r \in \mathbb{R}$

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

where we use that $|\xi(-t)| = \left|\overline{\xi(t)}\right| = |\xi(t)|$. Furthermore, by the definition of the characteristic function and using Fubini's theorem, we have that

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

Setting $z = y - x$, we get

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

where the identity $\sin x = (\exp(ix) - \exp(-ix))/2i$ was used. We proceed with the change of variable $v = rz$, giving

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

Using that $\sup_{x\in\mathbb{R}} |\sin x/x| < 1$, we have that $\prod_{k=1}^{p} \frac{2\sin(v_k)}{v_k} < 2^p$, leaving nested integrals of density functions over their entire support, which is equal to 1. This gives a finite upper bound on $\|\xi\|_{2j}^{2j}$ independent of r which concludes the proof for $q = 2j$. □

In the following sections, we will be interested in studying approximations to the characteristic function in terms of its Taylor approximation. As one might expect, computing the Fourier and inverse Fourier transforms of such approximations will involve computing the Fourier transforms of derivatives of the characteristic function. Before studying Fourier transforms of differential quatities, we introduce the notation that we will use in the rest of the thesis to express multivariate derivatives.

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

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

where $[p] = \{1, \ldots, p\}$. Let $f : \mathbb{R}^p \to \mathbb{R}$ be a k-times differentiable function, $s \in S_p(k)$ and $x_0 \in \mathbb{R}^p$, then the s-derivative of f in x_0 is given by

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

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

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

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

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

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

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

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

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

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

Iterating the previous steps completes the proof. □

A quantity related to the characteristic function and easier to manipulate is the *cumulant generating function*. 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

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

The derivatives of the cumulant generating function are called the *cumulants*. Let $s \in S_p(k)$ be an index vector of length k, then if the involved derivatives exist, we define the s-cumulant of X as

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

In the rest of the thesis, the cumulants might depend on various quantities (sample size, variable of interest, parameters of a distribution, ...) in which case we will use variations of this notation to make clear which cumulants are being discussed.

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

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

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

It is then clear that all cumulants of X exist, where first order cumulants are the components μ, second order cumulants are the components of Σ, and cumulants of higher order are 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 $s \in S(k)$

- $\kappa_s(X_1 + \ldots + X_n) = n\kappa_s(X_1)$
- For all $c \in \mathbb{R}$, $\kappa_s(cX_1) = c^k \kappa_s(X_1)$
- 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 $\kappa_s(Z)$ is the s-cumulant of the random variable Z.

One can see 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 also allows us to define the cumulants κ_s for $s \in S_p(k)$ in terms of the characteristic function

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

and hence

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

2.2 A heuristic introduction to the Edgeworth expansion

We now present a heuristic development of the idea behind the Edgeworth expansion. Consider two distributions P and Q over $\mathbb{R}^p$ with 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 a mean equal to 0 and a covariance matrix equal to $\mathbb{1}_p$. We wish to utilize the cumulants of both distribution to construct an approximation of P.

By formal expansion of the difference between the cumulant generating functions of P and Q around 0, we obtain 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 holds 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 $\alpha_s = \kappa_s - \gamma_s$, we can then continue by taking a formal expansion of the exponential function to find

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

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

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

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

$$\begin{aligned}
\alpha^*_{(k)} &= \alpha_{(k)} \\
\alpha^*_{(k,l)} &= \alpha_{(k,l)} + \alpha_{(k)}\alpha_{(l)} \\
\alpha^*_{(k,l,m)} &= \alpha_{(k,l,m)} + \alpha_{(k,l)}\alpha_{(m)} + \alpha_{(k)}\alpha_{(l)}\alpha_{(m)},
\end{aligned}$$

where the exact coefficient in front of the α terms are not relevant and ignored for conciseness. Coming back, by Lemma 2.4, we recognize the Fourier transform of derivatives of the density q of Q

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

which allows us to retrieve the density of P by Fourier inversion

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

A convenient choice for Q is the multivariate Normal distribution $\mathcal{N}_p(0, \mathbb{1}_p)$. Then, we have that the cumulants of P and Q of order $k = 1, 2$ of the two distributions match, implying $\alpha_s = 0$ for any $s \in S_p(k), k = 1, 2$. 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

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

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

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

Consider now applying this transformation to the standardized sum $Y = n^{-1/2} \sum_{i=1}^n X_i$ where $X_i \overset{iid}{\sim} P$. Then for any $s \in S_p(k)$, using properties of cumulants given in Lemma 2.6, the s-cumulants of Y are given by

$$\kappa_s(Y) = n^{1-k/2} \kappa_s(X_1) = o(n^{1-k/2}).$$

We can form the *Edgeworth series* of order k, called $e_k(y; \kappa(X))$, by discarding terms of order higher than $o(n^{1-k/2})$ in Equation (2.8), giving

$$f_Y(y) = e_k(y; \kappa(X)) + o(n^{(1-k)/2}). \tag{2.9}$$

Note that this statement can be slightly refined, which will be useful later. After truncating Equation (2.8), the density f can be decomposed in

$$f(y) = \phi(y) \left\{1 + P_k(y; \kappa(X)) + o(n^{(1-k)/2})\right\}, \tag{2.10}$$

where $P_k(\cdot; \kappa(X))$ 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, derivatives can only be taken with respect to a single variable and Equation (2.8) becomes

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

Let again Y be a standardized sum of n independent copies of X. To construct the Edgeworth approximation of order $k = 4$ to the density of Y, we truncate the above equation to only keep terms of size at least $o(n^{-1})$, that is we keep terms of size $o(n^{-1/2})$ and $o(n^{-1})$. 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 series

$$e_4(y;\kappa(X)) = \frac{1}{\sqrt{1\pi}} \exp\left(-\frac{y^2}{2}\right) \left\{1 + \frac{\kappa_3 H_3(y)}{6\sqrt{n}} + \frac{3\kappa_4 H_4(y) + \kappa_3^2 H_6(y)}{72n}\right\}. \tag{2.11}$$

While the argument provided above for the definition of the Edgeworth series is not suffenciently rigorous to prove Equation (2.9), we now show that the Edgeworth series $e_k(y;\kappa(X))$ 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 a mean of 0 and 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 $e_k(\cdot;\kappa(Z))$ can be constructed for the random variable $Z = \Sigma^{-1/2}(X-\mu)$ and used to construct an approximation $e_k(\cdot;\kappa(X))$ of the density of $n^{-1/2}\sum_{i=1}^n X_i$ via

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

In the rest of this thesis, we will 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 will implicitly make use of the change of variable formula mentioned in this remark.

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

Together with Remarks 2.8, this 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 of the Edgeworth approximation of order k is $o(n^{\lfloor (1-k)/2 \rfloor})$.

For instance, if $e_4(\cdot;\kappa(X))$ is Edgeworth expansion of order 4 from Example 2.7, we have

$$f_Y(y) = e_4(y;\kappa(X)) + \begin{cases} o(n^{-2}) & \text{if } y = 0 \\ o(n^{-3/2}) & \text{otherwise.} \end{cases}$$

2.3 Convergence of the Edgeworth expansion

While the previous section have provided an intuition for the development of the Edgeworth expansion, it is not a rigorous proof. In this section, we develop the a proof for the claims of the previous section.

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

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

In the following lemma, we relate how well z approximated $\exp u$ to how well v approximates u.

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

$$\left|\exp u - \sum_{k=0}^{l} \frac{v^k}{k!}\right| \leq \max\left\{\exp|u|, \exp|v|\right\} \left(|u-v| + \left|\frac{v^{l+1}}{(l+1)!}\right|\right). \tag{2.12}$$

Proof. By the triangle inequality,

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

Starting with the second term on the right hand side, we have

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

Furthermore, by Taylor's theorem there exists a point $z \in \mathbb{C}$ lying on the straight line between u and v such that

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

Taking absolute values and by convexity of the exponential function, we find the following bound

$$|\exp u - \exp v| = |u - v| \exp |z| \leq |u - v| \max \{\exp |u|, \exp |v|\} .$$

Combining the two bounds found previously completes the proof of the lemma. □

Continuing the development of the Edgeworth series, 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.

Theorem 2.11. Let ζ be the characteristic function of a random vector $X \in \mathbb{R}^p$ and let $n \in \mathbb{N}$. Assume that all cumulants of X of order up to $k \in \mathbb{N}$ exist and that the second cumulants of X satisfy $\kappa^{(i,j)} = \delta_{ij}$ for all $i, j = 1, \ldots, p$. Let

$$\xi(t) = \exp\left(-\frac{1}{2}\|t\|_2^2\right) \sum_{l=0}^{k-2} \frac{1}{l!} \left[1 + \sum_{m=3}^{k} \sum_{s \in S_p(m)} \frac{i^m \kappa_s t^s}{n^{m/2-1} m!}\right]^l . \tag{2.13}$$

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

$$\left|\zeta(tn^{-1/2})^n - \xi(t)\right| \leq \exp\left(-\frac{1}{4}\|t\|_2^2\right) \left[\frac{\epsilon \|t\|_2^k}{n^{k/2-1}} + \frac{C_p^{k-1} \|t\|_2^{3(k-1)}}{(k-1)! n^{k/2-1/2}}\right] \tag{2.14}$$

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 the Equation (2.14) to be able to use Lemma 2.10 and find suitable upper bounds on the remaining quantities. To that end, we define $u(t) = nu^*(tn^{-1/2})$ 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 can then rewrite

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

and

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

By Lemma 2.10, we can bound the left hand side of Equation (2.14) and have

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

We now continue to find suitable bounds on the resulting quantities. 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 $3 \le m < k$, then

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

where the derivative of the 2-norm of t is 0 because $|s| = m \ge 3$. Furthermore, we can compute the same derivatives of v^*,

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

The term $\frac{\mathrm{d}}{\mathrm{d}t_{s_1}}\cdots\frac{\mathrm{d}}{\mathrm{d}t_{s_m}}t_{s'_1}\ldots t_{s'_{m'}}|_{t=0} = 1$ if and only if s' is a permutation of s, otherwise 0. Hence

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

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

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

and if $\|t\| \le \delta\sqrt{n}$, this bound yields

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

Furthermore, choose δ 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

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

We observe that all derivatives of v^* in 0 of first and second order are equal to 0 and that the third 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 a δ small enough and $t \leq \delta\sqrt{n}$ we have

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

□

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 can finally prove the main theorem of this section by relating the approximation error of the Edgeworth density approximation to the error of the Edgeworth approximation to the characteristic function.

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

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

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

Proof. Without loss of generality, we assume that X_i has a mean equal to 0 and a covariance matrix equal to the identity, see Remark 2.8. Let ξ be the Fourier transform of $e_k(\cdot;\kappa)$, then by Corollay 2.2, we can bound the the absolute difference between f_Y and $e_k(\cdot;\kappa)$ as

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

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 parts in which t is small such that Theorem 2.11 can be used, and the rest of the integral will be handled separately.

By construction of the Edgeworth series, the Fourier transform of $e_k(\cdot;\kappa)$ corresponds to the function given in Equation (2.13) of Theorem 2.11. Hence, for any ε, there is a δ such that (2.14) holds and we can bound the *small* t part of the integral as

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

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 $\left\|t\right\|_2 \geq \delta\sqrt{n}$, we bound the integral by the triangle inequality and consider each term separately,

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

By construction of ξ, the integral I_1 has an exponential decay, faster than the $o(n^{(1-k)/2})$ we are trying to show. As for the integral I_2, using that $|\zeta(t)| < 1$ for $t \neq 0$ and $|\zeta(t)| \to 0$ for $n \to \infty$, there exists a $a \in (0,1)$ 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 a $q > 1$ 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 now investigate its behaviour when applied to an example for which the true density of the standardized sum is known.

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

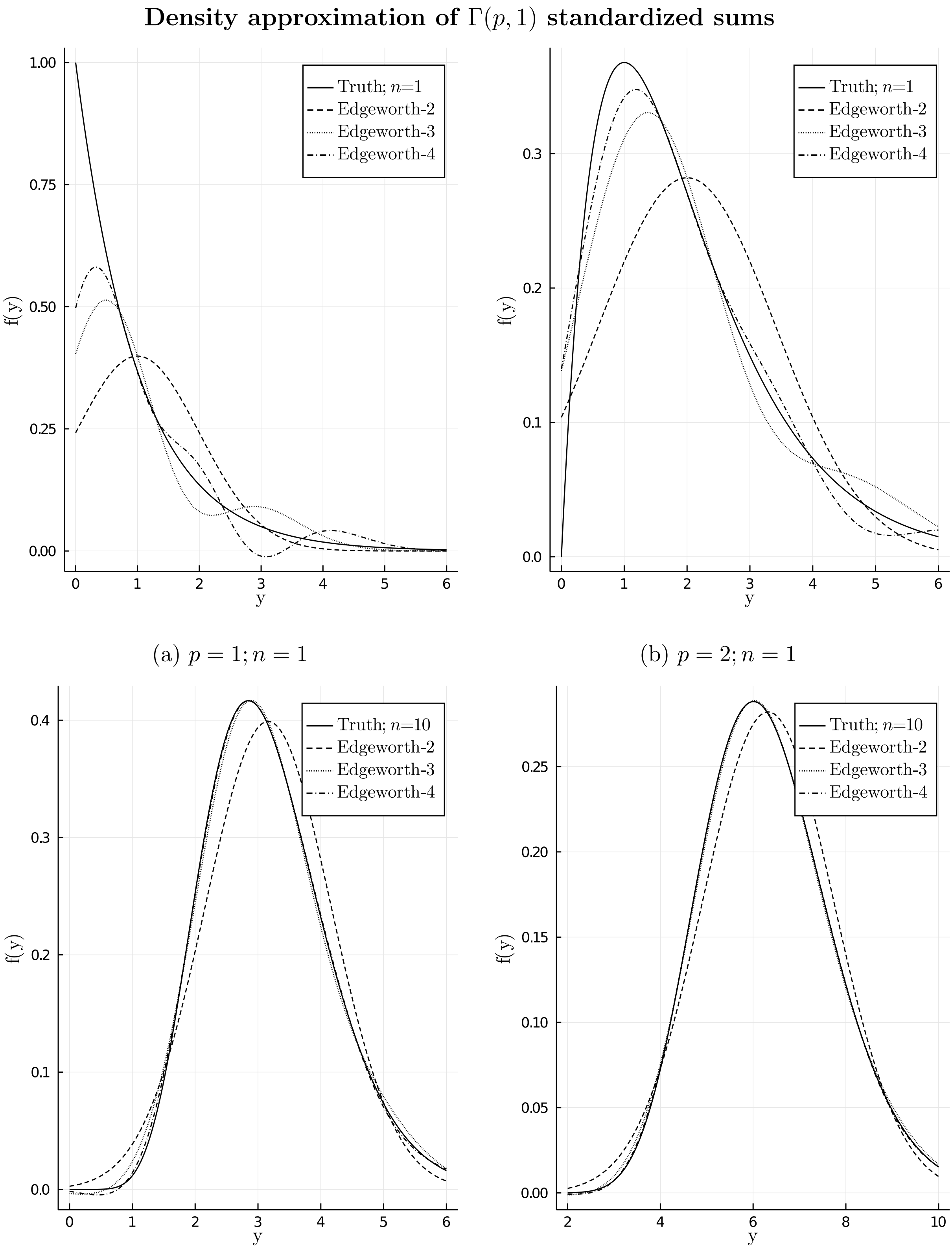
$$f(x) = \frac{\lambda^p}{\Gamma(p)} x^{p-1} \exp\left(-\lambda x\right),$$

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 the X_i follow Gamma distributions 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

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

hence the cumulant of order j 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.

We show several example of the behaviour of the Edgeworth approximation under differ-



(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 series approximation to the density of a standardized sum of n $\Gamma(p, 1)$ random variables.

ent conditions in Figure 1. In the upper pane of Figure 1, we compare the Edgeworth approximation of order $k = 2, 3, 4$ 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 $p = 1$, the $\Gamma(p, 1)$ is an exponential distribution. For $n = 1$, the discontinuity a $y = 0$ of the exponential distribution results in high oscillations of the Edgeworth series 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 approximate the $\Gamma(2, 1)$ distribution well. 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.

While Figure 1 seem to visually show good results of the approximation of the Edgeworth series, 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 $k = 2, 3, 4$ in approximating a standardized sum of $n = 10$ $\Gamma(p, 1)$ variables 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 panel 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.

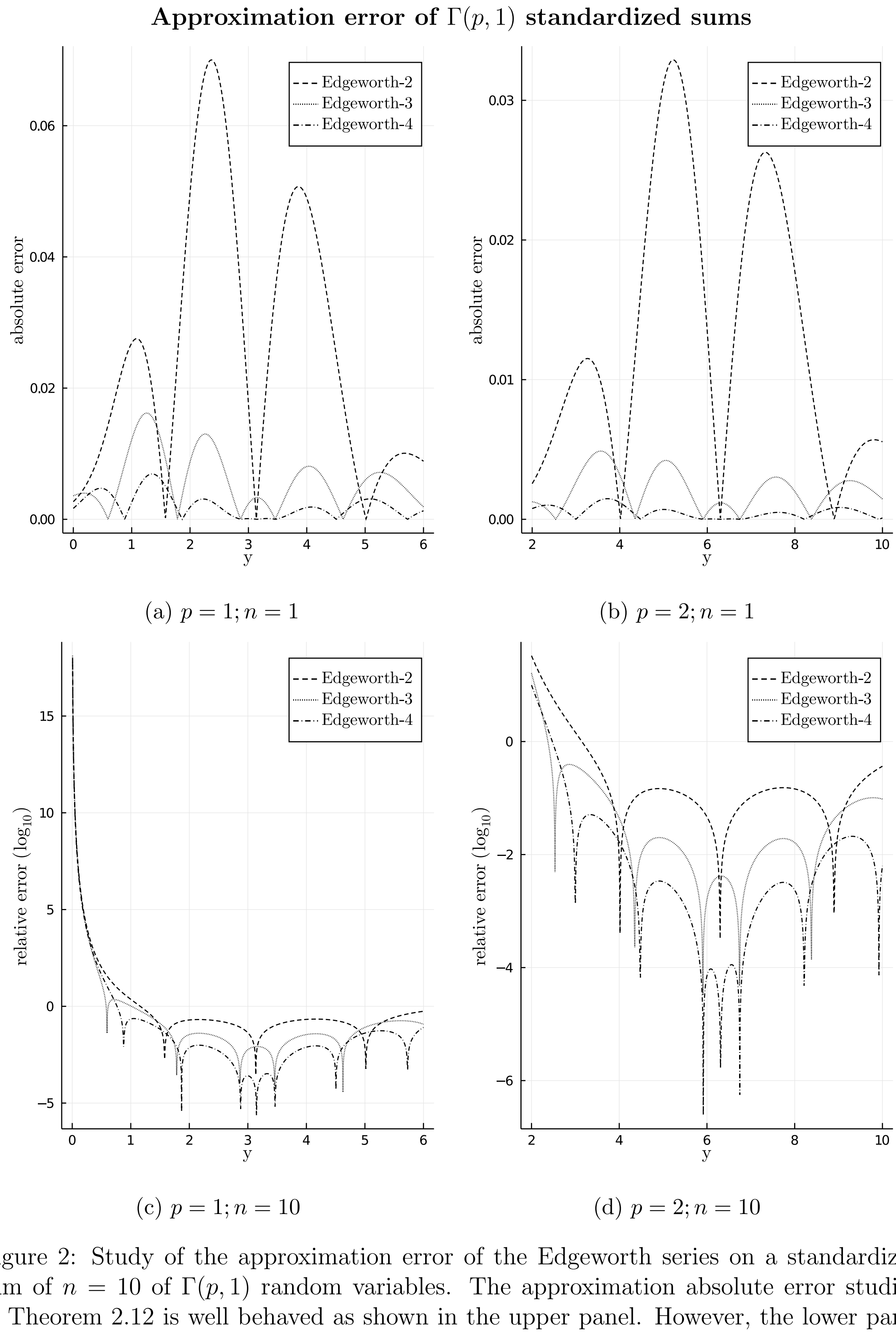
In many settings, one is interested in using distribution approximations to compute p-values in statistical tests. In this setting, one is trying to find statistical evidence against a null hypotheses by demonstrating a low p-value of the null hypothesis model. Hence, the Edgeworth series itself can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

2.5 Saddlepoint approximation

We now introduce another approach based on the Edgeworth series to create accurate density approximations that avoids some of the issues of the Edgeworth series that we have demonstrated in the previous section.

We now introduce the idea of *exponential tilting*. Consider a random random variable $X \in \mathbb{R}^p$ with cumulant generative 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_γ given by

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



(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 series on a standardized sum of $n = 10$ of $\Gamma(p, 1)$ random variables. The approximation absolute error studied in Theorem 2.12 is well behaved as shown in the upper panel. However, the lower panel 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.

Note that by the definition of the cumulant generating function, $K(\gamma)$ is the right normalization factor for $f(\cdot;\gamma)$ and hence $f(\cdot;\gamma)$ integrates to 1 and is a valid density function. Furthermore, the original distribution P is an element of $\mathcal{T}_P$ with $P = P_0$. Given two distributions in $\mathcal{T}_P$, their densities only differ by the factor $\exp\left(\gamma^\top x - K(\gamma)\right)$. Since the following holds for any $\gamma \in \mathbb{R}^p$

$$f(x) = f(x;\gamma)\exp\left(K(\gamma) - \gamma^\top x\right), \tag{2.15}$$

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 the cumulant generating function of S in Equation (2.15), we get

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

where $f_n(\cdot;\gamma)$ is the density of the mean of n i.i.d. random variables with density $f(\cdot;\gamma)$. 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 $\mu_\gamma, \Sigma_\gamma$ are the mean and covariance of $X_i \sim P_\gamma$. Furthermore, the determinant of the transformation is $n^{p/2}|\Sigma_\gamma|^{-1/2}$, which gives using the notation in Equation (2.10)

$$f_n(s;\gamma) = n^{p/2}|\Sigma_\gamma|^{-1/2}\phi(s^*)\left\{1 + P_k(s^*;\kappa(\gamma)) + o(n^{(1-k)/2})\right\}. \tag{2.16}$$

Furthermore, the cumulant generating function 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 of P_γ evaluated at 0, we have $\Sigma_\gamma = K''(\gamma)$. This lets us rewrite Equation (2.16) in terms of K as

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

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 second order Edgeworth approximation of even order gains half an order of accuracy 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 can now find a distribution $P_{\hat{\gamma}_s} \in \mathcal{T}_P$ with mean s by solving

$$K'(\hat{\gamma}_s) = s. \tag{2.17}$$

We choose to call the solution of this equation $\hat{\gamma}_s$ to emphasize the fact that instead of choosing one unique γ and then construct an approximation of the density of P_γ over $\mathbb{R}^p$, we find a different $\hat{\gamma}_s$ at each $s \in \mathbb{R}^p$ such that the Edgeworth approximation of the density of $P_{\hat{\gamma}_s}$ is accurate in s. Note that if $\hat{\gamma}_s$ solves (2.17), it is also the maximum likelihood estimator of γ within the model $\mathcal{T}_P$. Replacing $\hat{\gamma}_s$ in Equation (2.16), we get

$$f_n(s;\hat{\gamma}_s) = n^{p/2}(2\pi)^{-p/2}|\Sigma_{\hat{\gamma}_s}|^{-1/2}\left\{1 + P_k(0;\kappa(\hat{\gamma}_s)) + o(n^{\lfloor(1-k)/2\rfloor})\right\}.$$

Replacing this in the expression of f in terms of $f(\cdot;\hat{\gamma}_s)$ gives

$$\begin{aligned} f_n(s) &= \left(\frac{n}{2\pi}\right)^{p/2}\frac{\exp\left(nK(\hat{\gamma}_s/n) - \hat{\gamma}_s^\top s\right)}{|K''(\hat{\gamma}_s)|^{1/2}}\left[1 + P_k(0;\kappa(\hat{\gamma}_s)) + o(n^{\lfloor(1-k)/2\rfloor})\right] \\ &= g(s;K)\left[1 + P_k(0;\kappa(\hat{\gamma}_s)) + o(n^{\lfloor(1-k)/2\rfloor})\right] \end{aligned} \tag{2.18}$$

We call $g(\cdot;K)$ the *Saddlepoint approximation* to the density of S. We now justify the approximation accuracy claim from Equation (2.18) in the following theorem.

Theorem 2.14. Let P be a distribution with cumulant genrating function K and $k \in \mathbb{N}_{\geq 2}$ such that all cumulants of P of order up to k exist. Suppose that for every $s \in \mathbb{R}^p$, Equation (2.17) has a unique solution $\hat{\gamma}_s \in U$. Let $n \in \mathbb{N}$ and $X_1, \dots, X_n \overset{iid}{\sim} P$ and S be the mean

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

Then, if the density f_n of S exists, the expansion given in Equation (2.18) 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, the Remark 2.9 implies that only powers of n^{-1} have non-vanishing coefficients in the Edgeworth approximation of the tilted densities, which in turns implies that the Edgeworth approximation error in each point is of order $o(n^{\lfloor (1-k)/2) \rfloor})$. □

While the Saddlepoint approximation shows many advantages over the Edgeworth approximation, it is important to note that the Saddlepoint approximation uses information from the complete cumulant generating function of the approximated density. 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 is for $k = 2$. In this case, the Edgeworth approximation of $f_n(\cdot; \hat{\gamma}_s)$ is equal to its normal approximation and its polynomial part $P_k(\cdot; \kappa(\gamma))$ is equal to 0 and we get

$$\begin{aligned} f_n(s) &= g(s; K)\left[1 + o(n^{-1})\right] \\ &= \left(\frac{n}{2\pi}\right)^{p/2} \frac{\exp\left(nK(\hat{\gamma}_s/n) - \hat{\gamma}_s^\top s\right)}{|K''(\hat{\gamma}_s)|^{1/2}}\left[1 + o(n^{-1})\right] \end{aligned} \tag{2.19}$$

The Saddlepoint approximation of second order is commonly used in applications since it presents many advantages. It is has a simple expression which makes it easier to express it and manipulate it, 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. Continuing Example 2.13, we can analyze the behaviour of the Saddlpoint 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 (2.17), 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 order 3 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 panels show accurate approximation properties both in terms of relative and absolute error.

In this example, it is also interesting to examine the concrete form of the Saddlepoint approximation g_3. Replacing the relevant quantities in Equation (2.19), we obtain that the Saddlepoint approximation is

$$\begin{aligned} g_3(s;K) &= \sqrt{\frac{n}{2\pi K''(\lambda - \frac{p}{s})}} \exp\left(nK\left(\lambda - \frac{p}{s}\right) - n\left(\lambda - \frac{p}{s}\right)s\right) \\ &= \sqrt{\frac{n}{2\pi s^2/p}} \exp\left(n\left(p\log(\lambda) - p\log(p/s)\right) - ns\lambda + np\right) \\ &= (n\lambda)^{np} s^{np-1} \exp(-sn\lambda) \times \frac{(np)^{1/2-np}\exp(np)}{\sqrt{2\pi}}. \end{aligned}$$

Consider now the Stirling's formula for the gamma function

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

We recognize that the second term in the expression of $g_3(s;K)$ corresponds to the inverse of the Stirling's approximation to $\Gamma(np)$. The Saddlepoint approximation to the density of the mean of $\Gamma(p,\lambda)$ variables thus corresponds to the density of the true distribution $\Gamma(np, n\lambda)$ of the mean, where the gamma function has been replaced by the Stirling's approximation. This has the interesting 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 exposed in Figure 3 where the relative error of the Saddlepoint approximation is a straight horizontal line. Daniels [12] characterizes the class of distributions for which the uniform relative approximation error holds.

2.6 The p^* approximation in exponential families

Consider now applying the Saddlepoint approximation to an exponential family $\mathcal{P} = \{P_\theta\}_\theta$ with natural parameter $\theta \in \mathbb{R}^p$. The density f_θ of $P_\theta \in \mathcal{P}$ is given by

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

Given a random sample $x = (x_1, \ldots, x_n)$ of P_θ, the loglikelihood function is given by

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

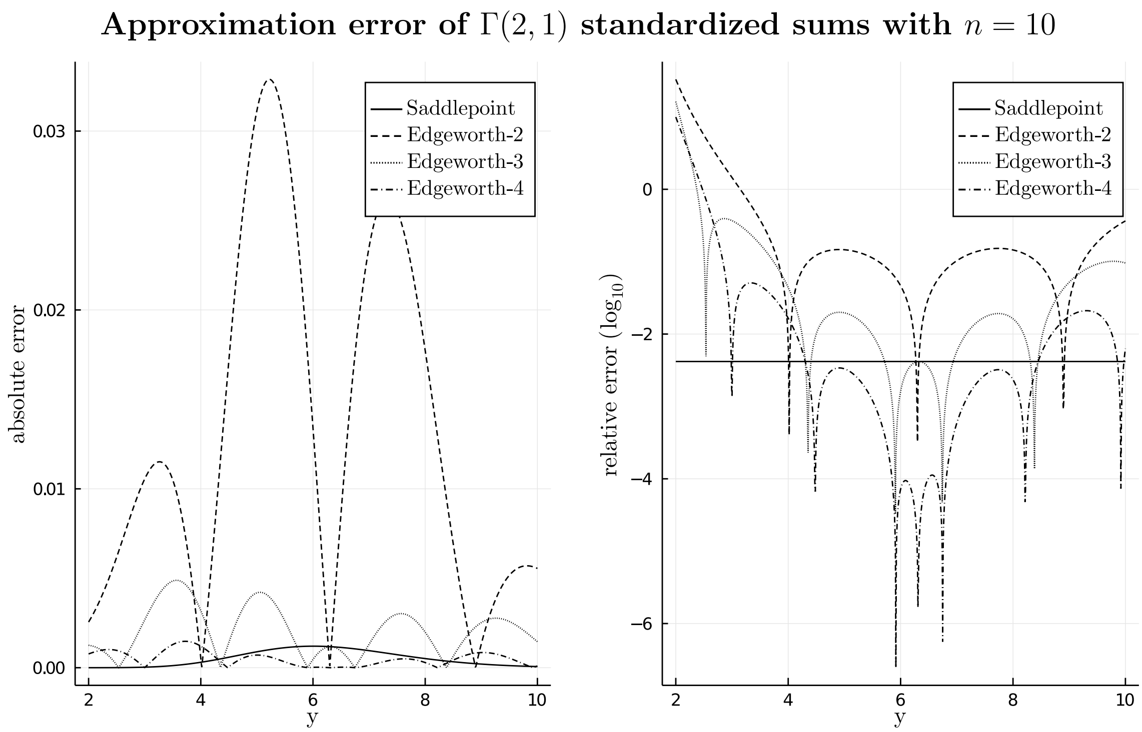


Figure 3: Study of the approximation error of the Saddlepoint approximation on a standardized sum of $n = 10$ of $\Gamma(2, 1)$ random variables. Both panel exposes properties studied of the Saddlepoint approximation: the accurate rellative error, the gain in order of approximation and the uniform relative error of the approximation for sums of Gamma random variables.

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

$$\mathcal{H}'(\hat{\theta}_{\bar{t}}) = \bar{t}. \tag{2.20}$$

For simplicity, we will assume that $\mathcal{H}'$ is one-to-one to ensure that (2.20) 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 $K_\theta(t) = \mathcal{H}(\theta + t) - \mathcal{H}(\theta)$ and thus $K'_\theta(t) = \mathcal{H}'(\theta + t)$. Using the cumulant generating function in the score equation gives

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

Considering the Saddlepoint equation given in (2.17), we notice that the parameter $\hat{\gamma}_{\bar{t}}$ of the tilted family nearly corresponds to the maximum likelihood estimator $\hat{\theta}$ with

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

Using this in the first order Saddlepoint approximation (2.19), we obtain that the Saddlepoint approximation for the average $\bar{T} = n^{-1}\sum_{i=1}^{n} T(X_i)$, (maybe justify that $T(X)$ is also in exp fam with same cgf and param, which is why the rest works) where $X_1, \dots, X_n \overset{iid}{\sim} P_\theta$, is

$$\begin{aligned}
g_3(\bar{t}; K_\theta) &= \left(\frac{n}{2\pi}\right)^{p/2} |K''_\theta(\hat{\theta}_{\bar{t}} - \theta)|^{-1/2} \exp\left(nK_\theta(\hat{\theta}_{\bar{t}} - \theta) - (\hat{\theta}_{\bar{t}} - \theta)^\top \bar{t}\right) \\
&= \left(\frac{n}{2\pi}\right)^{p/2} |\mathcal{H}''(\hat{\theta}_{\bar{t}})|^{-1/2} \exp\left(n(\mathcal{H}(\hat{\theta}_{\bar{t}}) - \mathcal{H}(\theta)) - (\hat{\theta}_{\bar{t}} - \theta)^\top \bar{t}\right) \\
&= \left(\frac{n}{2\pi}\right)^{p/2} |j(\hat{\theta}_{\bar{t}})|^{-1/2} \exp\left(\ell(\theta; \bar{t}) - \ell(\hat{\theta}_{\bar{t}}; \bar{t})\right),
\end{aligned}$$

where we have used 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 $\mathcal{H}'(\hat{\Theta}) = \bar{T}$, then, by change of variable, we can use the approximation above to construct an approximation p^* to the distribution of $\hat{\Theta}$,

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

To compute the determinant of the Jacobian of the transformation $\hat{\theta}(\bar{t})$, we can 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

$(\mathrm{d}\hat{\theta}/\mathrm{d}\bar{t}) = \mathcal{H}''(\hat{\theta})^{-1} = j(\hat{\theta})^{-1}$, giving

$$p^*(\hat{\theta};\theta,\bar{t}) = \left(\frac{n}{2\pi}\right)^{p/2} |j(\hat{\theta})|^{1/2} \exp\left(\ell(\theta;\bar{t}) - \ell(\hat{\theta};\bar{t})\right). \tag{2.21}$$

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 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 also highlights the fact that the p^* approximation inherited 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 situation where the distribution of refence is not necessarily an exponential family. It has been derived and studied in a much broader generality by a series of articles and books by Barndorff-Nielsen [2, 3].

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.*

Example 2.16. Consider now estimating the density of the maximum likelihood estimator of the parameter $\lambda \in \mathbb{R}_+$ of an exponential distribution. 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 Equation (2.21), we must work in the natural parametrization of the exponential distribution. For $\lambda \in R_+$, the corresponding natural parameter is $\theta = -\lambda \in \mathbb{R}_-$ and the density of $\mathrm{Exp}(\theta)$ is then $f_\theta(x) = \exp(\theta x + \log(-\theta))$.

Given a i.i.d. sample $x_1, \ldots, x_n$ of $\mathrm{Exp}(\theta)$, we have the likelihood

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

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 $j(\theta) = 1/\theta^2$. The p^* approximation to the density of $\hat{\theta}$ is then

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

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

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

Since $\mathrm{Exp}(\lambda) = \Gamma(1, \lambda)$, the distribution of $\bar{X}$ is $\Gamma(n, n\lambda)$ and hence $\hat{\lambda} = \bar{x}$ is Inv-$\Gamma(n, n\lambda)$. We can compare the p^* approximation to the commonly used Normal 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

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

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 compare these two approximations to the density of the MLE $\hat{\lambda}$ for $\lambda = 2$. As we can see in the left panel, 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 can 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 MLE, is the inverse of the sample mean $\bar{X}$, which is a diffeomorphic transformation for positive reals.

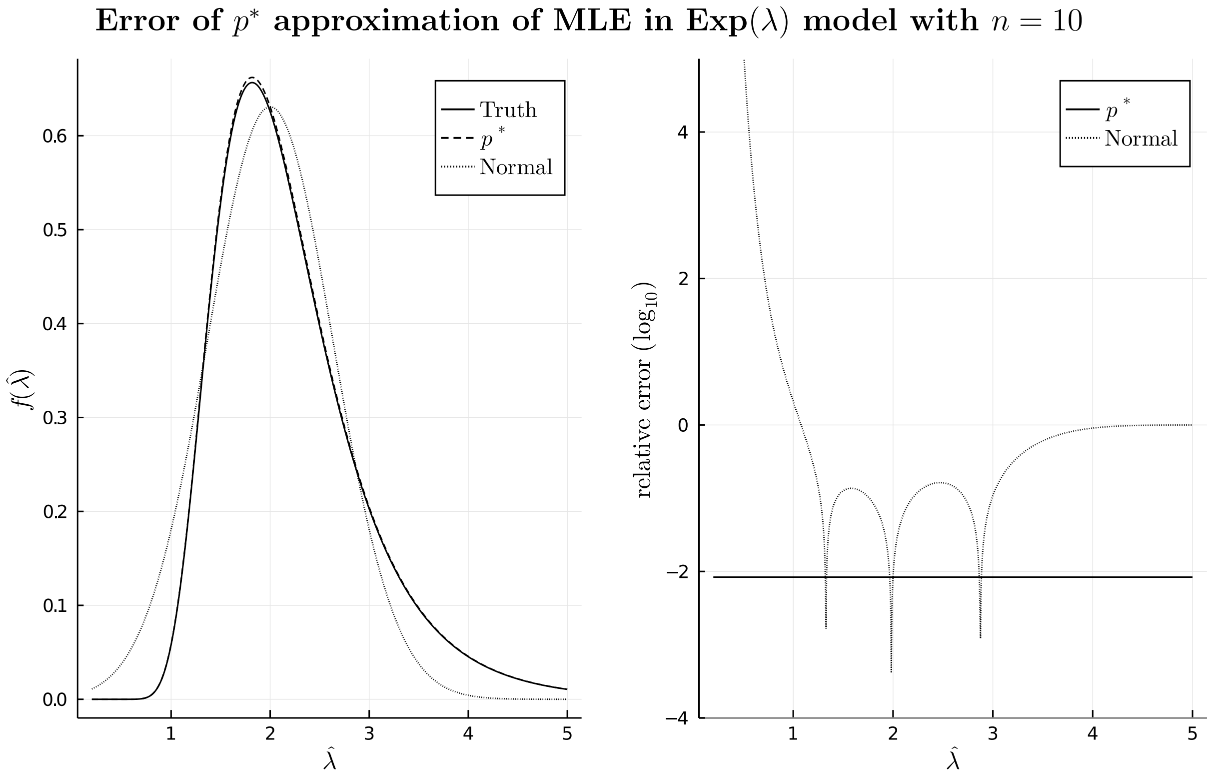


Figure 4: Study of the approximation error of the Saddlepoint approximation on a standardized sum of $n = 10$ of $\Gamma(2, 1)$ random variables. Both panel exposes properties studied of the Saddlepoint approximation: the accurate rellative error, the gain in order of approximation and the uniform relative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

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 [22]. 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 basic 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)(t)
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 together 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 instace, we can the code presented above 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, σ² = cumulants(gamma(p, λ), 2)
2-element Vector{Sym}:
   p/λ
   p/λ²
```

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 (TODO add ref) 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[1]

[1]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)
                                                              -x^2
                      /                                \      ---
                      |    κ_3^2 H_6(x)   κ_4 H_4(x)   κ_3 H_3(x)  |    2
0.398942280401433  |1 + ------ + ------ + ------- | e         2
                      |     72n         24n        6√n    |
                      \                                /
```

With $(2\pi)^{-1/2} \approx 0.398942280401433$, this formula corresponds expression derived in Equation (2.11) 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 Equation (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)
```

[2]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 Equation (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 the problems related to submodel selection in Gaussian graphical models. In Section (ref), we start with a review of 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 (ref), we apply the p^* approximation from Section (ref) 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 setting.

3.1 Preliminaries

We start by a brief introduction to elementary concepts in graph theory that will be useful in the rest of this chapter. Let $\mathcal{G} = (\Gamma, E)$ be a graph with nodes Γ and edges $E \subset \Gamma \times \Gamma$. We denote by $\mathrm{bd}(i)$ the set of *neighbours* of $i \in [p]$. For convenience, we will assume that the nodes are numbered and use $\mathcal{G} = ([p], E)$ and $E \subset [p] \times [p]$ for $p = |\Gamma|$. The graphs under study in this thesis will be unconnected and won't contain any loop. This lets us write edges using the set notation $e = \{i, j\}$ for $e \in E$. However, it will sometimes be useful to treat the set of edges as a set of indices on a matrix. In this case, we will need to introduce the *augmented edge set* to include indices refering to the diagonal entries of the matrix. The augmented edge set E^* of E is constructed by adding all possible loop in $\mathcal{G}$, $E^* = E \cup \{\{i\} : i \in \Gamma\}$.

A graph $\mathcal{G}$ is said to be *complete* if all pairs of distinct nodes are connected by an edge. A set of nodes $C \subset [p]$ is called a *clique* if the subgraph $\mathcal{G}_C = (C, E_C)$ with $E_C = \{\{i, j\} \in E : \{i, j\} \subset C\}$ is complete. We call $\mathcal{C}(\mathcal{G})$ the set of cliques in $\mathcal{G}$.

An important class of graphs are *chordal graphs*. A chordal graph $\mathcal{G}$ is a graph in which each cycle of length at least 4 has a *chord*, which is an edge which is not part of the cycle connecting two nodes in the cycle.

As mentioned before, edges will be used to index matrices. If $\mathcal{G} = ([p], E)$, 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 construced by keeping rows labeled by the entries in A and columns labeled by entries in B;
- If $C \subset [p]$, then $M_C = M_{C,C}$;

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

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

Since most matrices manipulated will be referencing quantities related to nodes in a graph, indexing of matrices and derived matrices will be done with respect to the nodes of the graph instead of row or column number of a matrix. For instance, if $A, B \subset [p]$ and $M \in \mathbb{R}^{p\times p}$, using the notation we just introduced, we have

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

3.2 MLE in Gaussian graphical models

A graphical model is a probabilistic models 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 $\Omega \in \mathcal{S}^p_{\succ 0}$ is the inverse of the *covariance matrix* Σ and is called the *precision matrix*. The density of X is then

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

We clearly see that the multivariate Gaussian distribution is an exponential family with canonical parameter Ω and sufficient statistic $\frac{1}{2}xx^\top$.

We choose to 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.

Lemma 3.1. Let $X \sim N_p(\mu, \Sigma)$ and let $i, j \in [p]$, then

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

Proof. By Lemma 3.8, 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 claim of this lemma 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

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

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

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

$$\Omega_{ij} = 0 \iff \{i, j\} \notin E. \tag{3.2}$$

This property corresponds to the pairwise Markov property in graphical model theory. All together, we find 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 following the presentation of Uhler [21, Section 9].

Consider now a sample $X = (X^1, \dots, X^n)$ from a Gaussian distribution. The log-likelihood function for a precision matrix $\Omega \in \mathcal{S}^p_{\succ 0}$ obtained from (3.1) is

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

Rewriting it in terms of the sufficient statistic $S = n^{-1} XX^\top$, we have

$$\ell(\Omega; S) = \frac{n}{2} \log |\Omega| - \frac{n}{2} \operatorname{tr}[S\Omega]. \tag{3.3}$$

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

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

However, 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 $\mathcal{S}(\mathcal{G})$ of $\mathcal{S}^p_{\succ 0}$ in which the conditional independence relations encoded in $\mathcal{G}$ are satisfied. This subset is directly given by Equation (3.2), $\mathcal{S}(\mathcal{G}) = \{\Omega \in \mathcal{S}^p_{\succ 0} : \Omega_{ij} = 0 \text{ if } i \neq$

j and $\{i,j\} \notin E\}$. We are then left with the following optimization problem

$$\begin{aligned} \underset{\Omega \in \mathcal{S}^p_{\succ 0}}{\text{maximize}} \quad & \log|\Omega| - \operatorname{tr}[S\Omega] \\ \text{subject to} \quad & \Omega \in \mathcal{S}(\mathcal{G}). \end{aligned} \tag{3.4}$$

Since the Gaussian graphical model condition is a linear constraint, the set $\mathcal{S}(\mathcal{G})$ is the is a convex cone. Showing that the objective function in (3.4) is concave would imply that maximum likelihood estimation in Gaussian graphical models is a convex optimization problem which would allow us to bring new insights to the problem by studying its dual formulation. We start by proving that the objective function is indeed concave.

Lemma 3.2. The function $f : \mathcal{S}^p_{\succ 0} \to \mathbb{R}, X \mapsto \log|X| - \operatorname{tr}[SX]$ is concave.

Proof. Since the sum of a linear function and a concave function is concave, and $\operatorname{tr}[SX]$ is linear in X, it is sufficient to show that the logarithm of the determinant of a matrix is a concave function. To do this, let us consider the line $\{U + tV : t \in \mathbb{R}\}$ for $U, V \in \mathcal{S}^p_{\succ 0}$. We can show that $X \mapsto \log|X|$ is concave on $\mathcal{S}^p_{\succ 0}$ by showing that $g(t) = \log|U + tV|$ is concave. Since $U \in \mathcal{S}^p_{\succ 0}$, both $U^{1/2}$ and $U^{-1/2}$ exist and we have

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

where λ_i are the eigenvalues of $U^{-1/2}VU^{-1/2}$ and we use that the eigenvalues of $1_p + tU^{-1/2}VU^{-1/2}$ are $1 + t\lambda_i$. Since each $\log(1 + t\lambda_i)$ is concave in t, we have that g is concave, completing the proof. □

We can now study the dual problem to (3.4). The Lagragian of the maximum likelihood estimation in Gaussian graphical models is

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

The Lagrange dual H of (3.4) is given by $H(\nu) = \mathcal{L}(\Omega^\nu, \nu)$ where Ω^ν is the maximizer of

$\mathcal{L}(\Omega, \nu)$. Derivating the expression of $\mathcal{L}(\Omega, \nu)$, we get that the inverse Σ^ν of Ω^ν satisfies

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

Note that Σ^ν is the matrix formed by replcing entries in S corresponding to missing edges with entries of the dual variables ν_{ij}. Replacing this in the expression for the Lagrange dual function H, we obain

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

And hence the dual to (3.4) is

$$\begin{aligned} &\underset{\Sigma \in \mathcal{S}^p_{\succ 0}}{\text{minimize}} \quad -\log|\Sigma| - p \\ &\text{subject to} \quad \Sigma_{ij} = S_{ij} \quad \text{for all } i = j \text{ or } \{i,j\} \in E \end{aligned} \tag{3.5}$$

To show that we can equivalently study problem (3.4) and (3.5), 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 $\mathcal{G}$ and we can freely study both formulations of the optimization problem. Furthermore, problems (3.4) and (3.5) have a solution if and only if $\log|\Sigma| + p$ is unbounded 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 new notation. If $\mathcal{G}$ is a graph over p nodes and $\Sigma \in \mathbb{R}^{p\times p}$, the $\mathcal{G}$-partial matrix $\Sigma^\mathcal{G}$ of Σ is the partial matrix found by removing entries in Σ corresponding to missing edges in $\mathcal{G}$, see Figure 5 for an example.With this notation, we can reformulate the dual problem (3.5) as

$$\begin{aligned} &\underset{\Sigma \in \mathcal{S}^p_{\succ 0}}{\text{minimize}} \quad -\log|\Sigma| - p \\ &\text{subject to} \quad \Sigma^\mathcal{G} = S^\mathcal{G}. \end{aligned} \tag{3.6}$$

If 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 [21, Section 9.4] presents a geometric argument tying together the matrix completion approach to the problem to its original convex optimization formulation.

Theorem 3.3. Consider a Gaussian graphical model associated to the graph $\mathcal{G}$ and a sample covariance matrix S. The maximum likelihood estimation 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 $\hat{\Omega} = \hat{\Sigma}^{-1}$.

Proof. This theorem is a reformulation of Theorem 9.4.2 in [21] in which $\mathcal{L} \cap \mathcal{S}^p_{\succ 0} = \mathcal{S}(\mathcal{G})$ which we have shown to contain at least 1_p. $\square$

We can 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. [17] introduce the *maximum likelihood threshold* of a graph $\mathcal{G}$, denoted $\mathrm{mlt}(\mathcal{G})$. The maximum likelihood treshold of a graph $\mathcal{G}$ is the smallest number of data points that guarantees that the maximum likelihood estimator exist almost surely in a Gaussian graphical model associated to the graph $\mathcal{G}$. In other words, $\mathrm{mlt}(\mathcal{G})$ is the smallest number of observations for which $S^{\mathcal{G}}$ can be 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 $\mathrm{rank}(S) = \min(n, p)$. Hence, if $n \geq p$, S itself is a valid positive completing for $S^{\mathcal{G}}$, giving the worst case bound

$$\mathrm{mlt}(\mathcal{G}) \leq p, \tag{3.7}$$

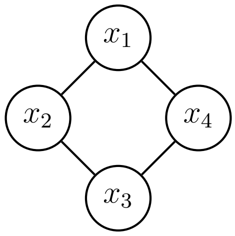
where equality holds if $\mathcal{G}$ is complete.

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 easily shown with the following argument: let $S^{\mathcal{G}}_{[p]\setminus I}$ be a principal completely specified submatrix of $S^{\mathcal{G}}$ such that there exists a $z \in \mathbb{R}^{p-|I|} \setminus \{0\}$ 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 $x_{-I} = 0$, 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 $S^{\mathcal{G}}$. Since $S^{\mathcal{G}}_{C}$ is complete, it is positive definite with probability one if and only if $n \geq |C|$. With

$q(\mathcal{G}) = \max \{|C| : C \text{ is a clique of } \mathcal{G}\}$ the maximum clique size in $\mathcal{G}$, we can lower bound the maximum likelihood threshold

$$q(\mathcal{G}) \leq \mathrm{mlt}(\mathcal{G}).$$

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



$$\underset{S^{\mathcal{G}}}{\begin{pmatrix} 1 & 0.9 & ? & -0.9 \\ 0.9 & 1 & 0.9 & ? \\ ? & 0.9 & 1 & 0.9 \\ -0.9 & ? & 0.9 & 1 \end{pmatrix}}$$

Figure 5: Example from [21, Section 9.3] of a matrix S for which all completely specified submatrices of $S^{\mathcal{G}}$ are positive definite but which doesn't have a positive definite completion.

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. [16] show that this condition is also sufficient exactly for chordal graphs.

Theorem 3.4. For a graph $\mathcal{G}$, the following statements are equivalent

(a) 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.

(b) $\mathcal{G}$ is chordal.

A consequence of this theorem is that if $\mathcal{G}$ is a chordal graph, $\mathrm{mlt}(\mathcal{G}) = q(\mathcal{G})$. 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 one in (3.7).

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 $S^{\mathcal{G}}$. Together with Theorem 3.4 to show the following bound

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

anda all together for any graph $\mathcal{G}$,

$$q(\mathcal{G}) \leq \text{mlt}(\mathcal{G}) \leq q^+(\mathcal{G}). \tag{3.8}$$

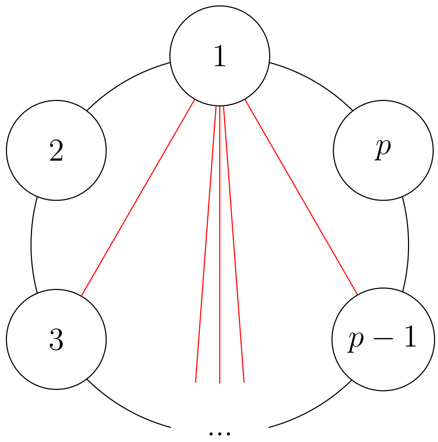


Figure 6: The graph $\mathcal{G} = ([p], E)$ formed from the black edges in the above figure is the cycle of length p. If E^+ is formed by adding the red edges in the figure to E, $\mathcal{G}^+ = ([p], E^+)$ forms a chordal cover of $\mathcal{G}$.

Example 3.5. Let $\mathcal{G} = ([p], E)$ be a chordless cycle of length $p \geq 4$, $E = \{(1,2),(2,3),\ldots,(p,1)\}$. The maximal clique size of $\mathcal{G}$ is $q(\mathcal{G}) = 2$ and it is clear that for any chordal cover $\mathcal{G}^+$ of $\mathcal{G}$, its maximal clique size is $q(\mathcal{G}^+) \geq 3$. We can form a chordal cover $\mathcal{G}^+ = ([p], \mathcal{G}^+)$ attaining the lower bound on $q(\mathcal{G}^+)$ by connecting an arbitrary node a to all other nodes of $\mathcal{G}$ that are not already a neighbour of a, $E^+ = E \cup \{(a,i) : i \in [p] \setminus \{a\}\}$. This chordal 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 $\hat{\Sigma}$ such that.

$$\hat{\Sigma}_C = S_C \quad \text{for all } C \in \mathcal{C}(\mathcal{G}). \tag{3.9}$$

This equation naturally suggests an iterative algorithm successively adjusting parts of the covariance matrix to satisfy (3.9) while keeping the running matrix positive definite. This procedure, called *iterative proportional scaling*, was studied by Speed and Kiiveri [23] among with other algorithms for solving the maximum equation problem in a Gaussian graphical model.

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

$$T_C\Omega = \Omega + \begin{pmatrix} (S_C)^{-1} - (\Sigma_C)^{-1} & 0 \\ 0 & 0 \end{pmatrix}, \tag{3.10}$$

where the variable Σ will be used to denote the inverse of Ω and, for simplicity of notation, we will use that the top-left block of matrices writen out explicitly corresponds to the current clique C. We now show that the operator T_C has the following useful properties.

Proposition 3.6. The operator T_C satisfies

(i) T_C is well defined;

(ii) T_C adjusts the C-marginal of Ω, that is, $(T_C\Omega)^{-1}$ satisfies Equation (3.9) for the clique C;

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

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

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 completement

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

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

$$T_C\Omega = \begin{pmatrix} (S_C)^{-1} + \Omega_{C,C^c}(\Omega_{C^c})^{-1}\Omega_{C^c,C} & \Omega_{C,C^c} \\ \Omega_{C^c,C} & \Omega_{C^c,C^c} \end{pmatrix}. \tag{3.11}$$

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) By Lemma 3.9, $T_C\Omega$ 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), $(T_C\Omega)_C = S_C$ and is by assumption positive definite. As for the Schur 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 an missing edge in $\mathcal{G}$. Then, 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 by T_C, we have that $(T_C\Omega)_{ij} = \Omega_{ij} = 0$ and 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 adjustement 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 adjustement operator computes the solution to a contrained version of (3.4).

Lemma 3.7. Let $\Omega^0 \in \mathcal{S}_{\succ 0}(\mathcal{G})$, the C-marginal adjustement operator T_C computes the solution to problem (3.4) over the section

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

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 Ω^0 = 1_p
2: Let Ω^1 = Ω^0
3: for C ∈ C(G) do
4:     Set Ω^1 := T_C Ω^1
5: end for
6: if ||Ω^1 − Ω^0|| < ε then
7:     Return Ω̂ := Ω^1
8: else
9:     Set Ω^0 := Ω^1
10:    Go to line 2.
11: end if
```

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

$$\begin{aligned} &\underset{\Omega\in\mathcal{S}_{\succ 0}(\mathcal{G})}{\text{maximize}} \quad \log|\Omega| - \mathrm{tr}[S\Omega] \\ &\text{subject to} \quad \Omega_{C^c} = \Omega^0_{C^c} \text{ and } \Omega_{C,C^c} = \Omega^0_{C,C^c}. \end{aligned} \tag{3.12}$$

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

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

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

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

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 (3.12), it can be ignored and we have $\log|\Omega| \doteq \log|\Omega'|$, where $\doteq$ denotes equality up to a constant term. Furthermore, using again that $\Omega \in \Theta_C(\Omega^0)$, we have

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

Hence, the optimization problem (3.12) is equivalent to

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

Comparing this to earlier discussions, this problem is equivalent to finding the maximum likelihood estimator of the precision matrix Ω' in 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 (3.12) is given by $\hat{\Omega} \in \Theta(\Omega^0)$ with

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

and hence the solution to (3.12) is $\hat{\Omega} = T_C\Omega^0$. □

Hence, Algorithm 1 corresponds to an *iterative partial maximization* algorithm, or block coordinate descent algorithm. Since T_C is a linear transformation, it is continuous and we have already shown that T_C maps $\mathcal{S}_{\succ 0}(\mathcal{G})$ onto itself. With these assumptions satisfied, Lauritzen [20, Proposition A.3] shows that the iterative partial maximization algorithm converges and hence, Algorithm 1 converges to the maximum likelihood estimator $\hat{\Omega} \in \mathcal{S}_{\succ 0}(\mathcal{G})$.

Lemma 3.8. 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

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

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

Proof. See [20, Proposition C.5] □

Lemma 3.9. Let $\Sigma \in \mathcal{S}^p$ be a symmetric block diagonal matrix decomposing as

$$\Sigma = \begin{pmatrix} A & B \\ B^\top & C \end{pmatrix}.$$

Then, $\Sigma \in \mathcal{S}^p_{\succ 0}$ if and only if both $E = A - BC^{-1}$ and C are positive definite.

Proof. See [20, Proposition B.1] □

3.3 Hypothesis testing

We now turn ourselves to applying the approximations developed in Section (todo) on 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 problem

$$H_0 : \Omega \in \mathcal{S}_{\succ 0}(\mathcal{G}_0) \quad \text{vs.} \quad H_1 : \Omega \in \mathcal{S}_{\succ 0}(\mathcal{G}) \setminus \mathcal{S}_{\succ 0}(\mathcal{G}_0). \tag{3.13}$$

Lemma 3.10. [15] Let $\mathcal{G}$ be a graph, $\Omega \in \mathcal{S}_{\succ 0}(\mathcal{G})$ and S be a sample covariance matrix computes from a sample of size n of the Gaussian graphical model associated to $\mathcal{G}$ with precision matrix Ω. Then, the density $p(S;\Omega)$ of S satisfies

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

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

$$j_{\mathcal{G}}(\Omega)_{ab} = \mathrm{tr}\left[\Omega^{-1}H_a\Omega^{-1}H_b\right] \text{ for all } a, b \in E. \tag{3.14}$$

Proof. Since $XX^\top$ is sufficient in the Gaussian graphical model, S corresponds to the sample average of the sufficient statistic. Applying the Saddlepoint approximation to S as done in Section (todo), we have that the density of S satisfies

$$p(S;\Omega) = c|j_{\mathcal{G}}(\hat{\Omega}_{\mathcal{G}}(S))|^{-1/2} \exp\left\{\ell(\Omega;S) - \ell(\hat{\Omega}_{\mathcal{G}}(S);S)\right\}(1 + O(n^{-3/2})).$$

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

$$\begin{aligned}
p(S;\Omega) &\propto |j_{\mathcal{G}}(\hat{\Omega}_{\mathcal{G}}(S))|^{-1/2} \exp\left\{\ell(\Omega;S) - \ell(\hat{\Omega}_{\mathcal{G}}(S);S)\right\}(1 + O(n^{-3/2})) \\
&\propto |j_{\mathcal{G}}(\hat{\Omega}_{\mathcal{G}}(S))|^{-1/2}\frac{|\Omega|^{n/2}}{|\hat{\Omega}_{\mathcal{G}}(S)|^{n/2}} \exp\left\{-\frac{n}{2}\left(\mathrm{tr}\left[\Omega S\right] - \mathrm{tr}\left[\hat{\Omega}_{\mathcal{G}}(S)S\right]\right)\right\}(1 + O(n^{-3/2})) \\
&\propto |j_{\mathcal{G}}(\hat{\Omega}_{\mathcal{G}}(S))|^{-1/2}\frac{|\Omega|^{n/2}}{|\hat{\Omega}_{\mathcal{G}}(S)|^{n/2}} \exp\left\{-\frac{n}{2}\mathrm{tr}\left[\Omega S\right]\right\}(1 + O(n^{-3/2}))
\end{aligned}$$

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

Consider now a Gaussian graphical model with graph $\mathcal{G} = ([p], E)$ and the sub-model constructed by remove an edge $a \in E$ from $\mathcal{G}$. The sub-model is then the Gaussian graphical model associated to the graph $\mathcal{G}_0 = ([p], E_0)$ where $E_0 = E \setminus \{e_0\}$. Without loss of generality, we assume $e_0 = \{1, 2\}$. Let S be the sample covariance matrix and assume that the true parameter is $\Omega_0 \in \mathcal{S}_{\succ 0}(\mathcal{G}_0)$. We can then construct approximations to the densities $p(S^{\mathcal{G}_0}; \Omega_0)$ and $p(S^{\mathcal{G}}; \Omega_0)$ by applying Lemma 3.10 in the Gaussian graphical models associated to $\mathcal{G}$ and $\mathcal{G}_0$ to get

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

and

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

Combining these results together allows us to approximate the density of S_e conditioned on $S^{\mathcal{G}_0}$

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

where we used in the last step that $\Omega_0 S^{\mathcal{G}} = \Omega_0 S^{\mathcal{G}_0}$ which leads to the exponential terms canceling out. Since $w \xrightarrow{d} \chi_1^2$ is asymptotically ancillary, and $q = \exp\left\{-\frac{1}{2}w\right\}$, q is also asymptotically ancillary. Since $S^{\mathcal{G}_0}$ is a complete sufficient statistic assuming $\mathcal{G}_0$, $S^{\mathcal{G}_0}$ and q are asymptotically independent by Basu's Theorem [6]. This means 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. Taking $S^{\mathcal{G}_0} = 1_p$ gives

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

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

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

for some normalizing constant $\hat{c}$.

We now focus our attention to computing the determinant of the observed information matrix given in (3.14) 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 $\{i\} \cup \{\bar{i}\} = b$. Using this in the expression of $j_{\mathcal{G}}(S)_{ab}$, we get

$$\operatorname{tr}[SH_aSH_b] = \sum_{i=1,j=1}^{p} (SH_a)_{ij}(SH_b)_{ji} = \sum_{(i,j)\in a\times b} S_{i\bar{j}}S_{j\bar{i}} = \sum_{e\in a\times b} S_e S_{\bar{e}}, \tag{3.15}$$

where the last equality only involves re-indexing and re-ordering the sum. We now inspect the different a, b for which the summand $S_e S_{\bar{e}}$ is non-zero. Since we chose $S = 1_p + sH_{e_0}$, we have that

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

Hence the summands $S_e S_{\bar{e}}$ of (3.15) 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 will assume that $e_0 = \{1, 2\}$. This leaves us with the following cases.

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

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

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

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

since we assumed that $S = 1_p + sH_{e_0}$.

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 we get

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

since $S_{ii} = 1$, $S_{1,2} = s$ and $S_{i1} = S_{i2} = 0$. Note that since the matrix $j_{\mathcal{G}}$ is indexed by edges in $\mathcal{G}$, the cases $a = \{1,i\}$ and $b = \{2,i\}$ are only relevant if $a,b \in E$ and so this case only for $i \in C = \mathrm{bd}(1) \cap \mathrm{bd}(2)$.

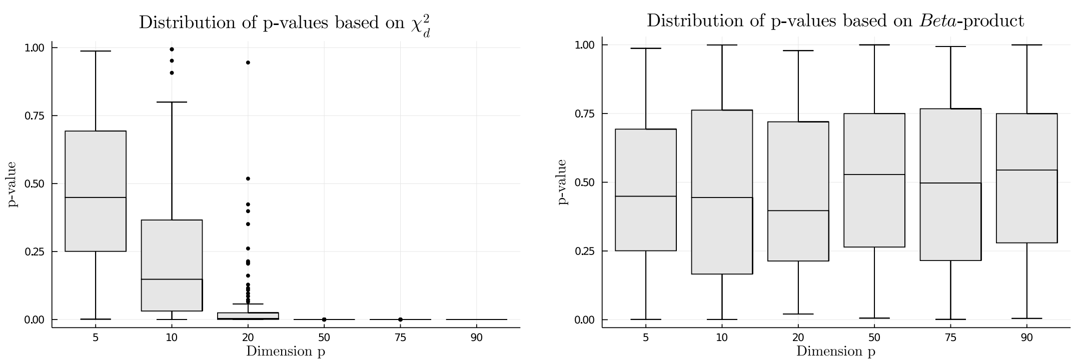
Case 4. $e = \{i\}$ and $\bar{e} = \{j\}$. This only happens is $a = b = \{i,j\}$, which, again using that $a,b \in E$ and $S = 1_p + sH_{e_0}$ gives

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

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

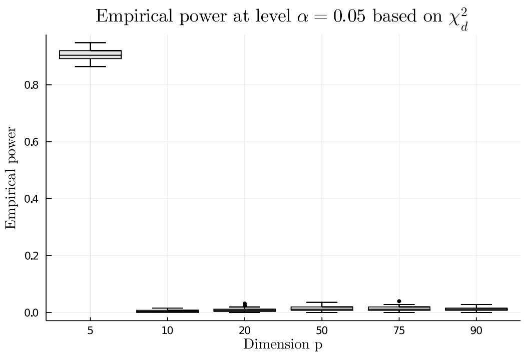
$$A = \begin{array}{c} \\ \{1\} \\ \{2\} \\ \{1,2\} \end{array} \begin{array}{c} \begin{array}{ccc} \{1\} & \{2\} & \{1,2\} \end{array} \\ \begin{pmatrix} 1 & s^2 & 2s \\ s^2 & 1 & 2s \\ 2s & 2s & 2+2s^2 \end{pmatrix} \end{array} \qquad B_i = \begin{array}{c} \\ \{1,i\} \\ \{2,i\} \end{array} \begin{array}{c}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

Since $|A| = 2(1-s)^3$ and $|B_i| = 4(1-s)$ for $i \in C$, we have that the determinant of the observed information $|j_{\mathcal{G}}(1_p + sH_{e_0})| \propto (1-s)^{3+|C|}$.

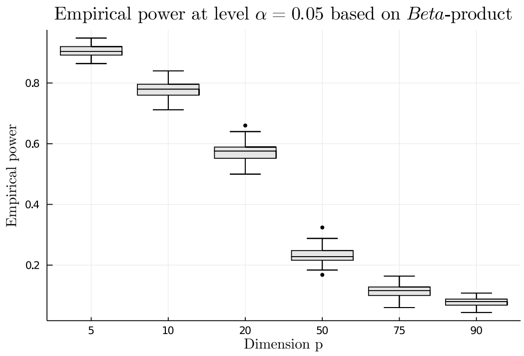


(a) (b)

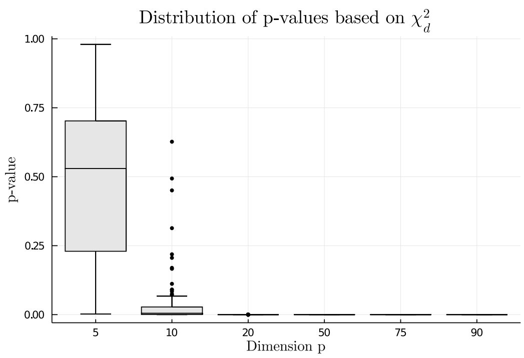
[24]


Empirical power at level $\alpha = 0.05$ based on χ^2_d
Empirical power
0.0
0.2
0.4
0.6
0.8
5
10
20
50
75
90
Dimension p

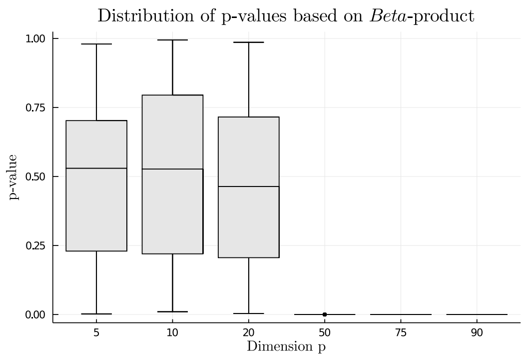
(a)


Empirical power at level $\alpha = 0.05$ based on *Beta*-product
Empirical power
0.2
0.4
0.6
0.8
5
10
20
50
75
90
Dimension p

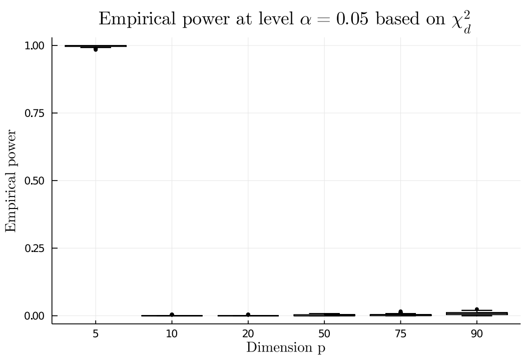
(b)


Distribution of p-values based on χ^2_d
p-value
0.00
0.25
0.50
0.75
1.00
5
10
20
50
75
90
Dimension p

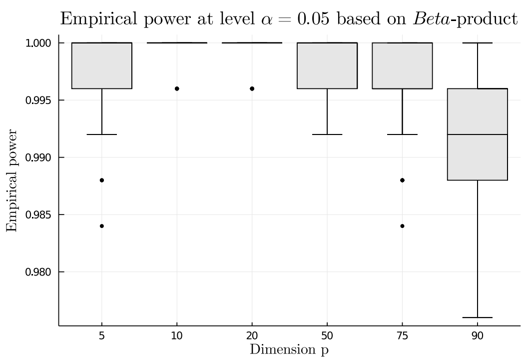
(a)


Distribution of p-values based on *Beta*-product
p-value
0.00
0.25
0.50
0.75
1.00
5
10
20
50
75
90
Dimension p

(b)


Empirical power at level $\alpha = 0.05$ based on χ^2_d
Empirical power
0.00
0.25
0.50
0.75
1.00
5
10
20
50
75
90
Dimension p

(a)


Empirical power at level $\alpha = 0.05$ based on *Beta*-product
Empirical power
0.980
0.985
0.990
0.995
1.000
5
10
20
50
75
90
Dimension p

(b)

We now compare different properties of the hypothesis test based on the χ^2_d approximation to the likelihood ratio and the product of Beta distributions described in (todo ref). 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 keeping the probability of making a false discovery under control.

Evaluating the size of a test is equivalent to evaluating the quality of the asymptotic distribution approximation used by the test in finite sample.

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