Asymptotic accuracy of the saddlepoint approximation for maximum likelihood estimation

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Abstract

The saddlepoint approximation gives an approximation to the density of a random variable in terms of its moment generating function. When the underlying random variable is itself the sum of \( n \) unobserved i.i.d. terms, the basic classical result is that the relative error in the density is of order \( 1/n \). If instead the approximation is interpreted as a likelihood and maximized as a function of model parameters, the result is an approximation to the maximum likelihood estimator (MLE) that is often much faster to compute than the true MLE. This paper proves the analogous basic result for the approximation error between the saddlepoint MLE and the true MLE: it is of order \( 1/n^2 \).

The proof is based on a factorization of the saddlepoint likelihood into an exact and approximate term, along with an analysis of the approximation error in the gradient of the log-likelihood. This factorization also gives insight into alternatives to the saddlepoint approximation, including a new and simpler saddlepoint approximation, for which we derive analogous error bounds. In addition, we prove asymptotic central limit theorem results for the sampling distribution of the saddlepoint MLE and for the Bayesian posterior distribution based on the saddlepoint likelihood. Notably, in the asymptotic regime that we consider, the difference between the true and approximate MLEs is negligible compared to the asymptotic size of the confidence region for the MLE. In particular, the true MLE and the saddlepoint MLE have the same asymptotic coverage properties, and the saddlepoint MLE can be used as a readily calculated substitute when the true MLE is difficult to compute.

1 Introduction

Let \( X \) be a random variable with density function \( f(x), x \in \mathbb{R} \). Define

\[
M(s) = \mathbb{E}(e^{sx}), \quad K(s) = \log M(s),
\]

the moment generating function (MGF) and cumulant generating function (CGF), respectively, associated to \( X \). Given \( x \in \mathbb{R} \), let \( \hat{s} \) be the solution to

\[
K'(\hat{s}) = x
\]

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and set
\[ \hat{f}(x) = \frac{\exp(K(\hat{s}) - \hat{s}x)}{\sqrt{2\pi K''(\hat{s})}}. \]  
(1.3)

We call \( \hat{f}(x) \) the saddlepoint approximation to the density function \( f(x) \).

Thinking of \( f(x) \) as our object of study, we are led to ask how well \( \hat{f}(x) \) approximates \( f(x) \) as a function of \( x \). For instance, we may naturally ask whether the ratio \( \hat{f}(x)/f(x) \) tends to 1 in a suitable limit, and how fast this convergence occurs. The most prominent results of this kind concern what we will call the standard asymptotic regime, in which the observed value \( X \) is the sample average of \( n \) i.i.d. (but unobserved) values. We describe this limiting setup in greater detail in Section 2.2. In the standard asymptotic regime, the classical basic result is that \( \hat{f}(x)/f(x) \to 1 \) as \( n \to \infty \) (for a precise statement of this kind, see [6] or Proposition 15 below). This convergence justifies our description of \( \hat{f}(x) \) as an approximation to \( f(x) \). Moreover the limit comes with a rate of convergence estimate, \( \hat{f}(x)/f(x) = 1 + O(1/n) \) as \( n \to \infty \).

A notable advantage of the saddlepoint approximation is that, under many circumstances, the ratio \( \hat{f}(x)/f(x) \) is uniformly bounded, even near the boundary of the support of \( X \): see [13, Theorem 4.6.1] and [11]. Under stronger assumptions including that the true density is log-concave, the ratio \( \hat{f}(x)/f(x) \) tends to 1 near the boundary [2]. Thus the saddlepoint approximation correctly captures the behaviour of the density in the tails. This is in marked contrast to other density approximations such as normal approximations or Edgeworth expansions, which immediately extrapolate to an unbounded support with Gaussian-like tails even when the underlying random variable has values lying in a compact set.

On the other hand, the saddlepoint approximation does not produce a normalised density function. Thus, for instance, we cannot straightforwardly apply the saddlepoint approximation to obtain a random variable \( \hat{X} \) whose distribution approximates the distribution of \( X \).

In this paper, we shift perspectives and consider (1.3) as an approximation to the likelihood. That is, we now consider \( X \) to have a parameter \( \theta \) and write the density and CGF as \( f(x; \theta), K(s; \theta) \) to emphasise their dependence on the parameter. Instead of (1.3) we write
\[ \hat{L}(\theta; x) = \frac{\exp(K(\hat{s}; \theta) - \hat{s}x)}{\sqrt{2\pi K''(\hat{s}; \theta)}}, \]  
(1.4)
the saddlepoint approximation to the likelihood \( L(\theta; x) = f(x; \theta) \). Note that the saddlepoint \( \hat{s} = \hat{s}(\theta; x) \) is a function of both the parameter \( \theta \) and the observed value \( x \), defined implicitly by
\[ K'(\hat{s}; \theta) = x \]  
(1.5)
and the derivatives \( K', K'' \) are with respect to \( s \).

In this perspective, we think of \( x \) as fixed and examine the dependence of \( \hat{L}(\theta; x) \) on the parameter \( \theta \). In particular, we can form the saddlepoint maximum likelihood estimator (MLE)
\[ \hat{\theta}_{\text{MLE}}(x) = \arg\max_\theta \hat{L}(\theta; x) \]  
(1.6)
corresponding to an observed value \( x \). We then wish to quantify the accuracy of \( \hat{\theta}_{\text{MLE}}(x) \) compared to the true MLE
\[ \theta_{\text{MLE}}(x) = \arg\max_\theta L(\theta; x). \]  
(1.7)
A central result of this paper is that the MLE approximation error, $|\hat{\theta}_{\text{MLE}}(x) - \theta_{\text{MLE}}(x)|$, is asymptotically of order $1/n^2$.

Outline of the paper Section 2.1 introduces further notation, including conventions for vectors and gradients. In Section 2.2, we formulate the standard asymptotic regime as an explicit limiting framework relating the distribution $X_\theta$, its CGF $K$, the observed value $x$, and the parameter $n$. The main results, Theorems 1–5, are stated in Section 2.3. Section 2.4 explores how these results apply in several examples, including simple distributions and examples from the literature. We also explain why the saddlepoint MLE is always exact for exponential families. Section 2.5 gives further general discussion.

Section 3 sets the stage for the proofs by exploring in more detail how the saddlepoint approximation arises. In particular, Section 3.1 expresses the saddlepoint procedure as a combination of an exact step (tilting) and an approximation step, and introduces a factorisation and reparametrisation of the likelihood that underlies the rest of the paper. As a by-product, we obtain in Section 3.2 a “lower-order” version of the saddlepoint approximation, satisfying analogues of the main results with a different power of $n$.

The proofs of Theorems 1–2 are given in Section 4, along with a summary in Section 4.1 of gradients of quantities related to the saddlepoint approximation. Further proofs and technical details appear in Appendices A–G.

Section 5 includes a summary, additional discussion, and directions for further inquiry.

2 Main results

2.1 Setup and notation

2.1.1 Moment and cumulant generating functions

We consider a vector-valued random variable $X$ of dimension $m$ depending on a parameter $\theta$ of dimension $p$, and write $X = X_\theta$ to indicate the dependence. We consider the values of $X_\theta$ and $\theta$ to be column vectors, i.e., $m \times 1$ or $p \times 1$ matrices, which we express as $X_\theta \in \mathbb{R}^{m \times 1}, \theta \in R \subset \mathbb{R}^{p \times 1}$ where $R$ is an open subset of $\mathbb{R}^{p \times 1}$. The multivariate MGF and CGF are

$$ M(s; \theta) = \mathbb{E}(e^{sX_\theta}), \quad K(s; \theta) = \log M(s; \theta). \quad (2.1) $$

At times we will omit the dependence of $M, K$ on $\theta$ and write simply $M(s), K(s)$. On those occasions when we consider more than one random variable, we will write $M_X, M_Y$ and so on to distinguish the respective generating functions.

In (2.1), $s$ is called the dual variable to $X$, and we interpret it as a row vector, a $1 \times m$ matrix, so that $sX$ is a scalar or $1 \times 1$ matrix. This convention emphasises that $s$ and $X$, despite being vectors of the same dimension, play quite different roles and are not interchangeable; rather, the space of row vectors is the natural dual space to the space of column vectors. This convention also avoids excessive use of transposes and explicit inner products.

We wish to consider $M$ and $K$ for complex-valued $s$, and to this end we must take care of convergence issues in (2.1). Let

$$ S_\theta = \{ s \in \mathbb{R}^{1 \times m} : \mathbb{E}(e^{sX_\theta}) < \infty \}, \quad S = \{(s, \theta) : s \in S_\theta \}. \quad (2.2) $$

Writing $\text{Re}(z)$ for the real part of the complex number $z$, we have $|e^z| = e^{\text{Re}(z)}$ for $z \in \mathbb{C}$. Hence the expectation in (2.1) converges absolutely whenever $\text{Re}(s) \in S_\theta$, and we
take the domain of $M$ to be $\{ (s, \theta) \in \mathbb{C}^{1 \times m} \times R : \text{Re}(s) \in S_\theta \}$. Here we interpret $\text{Re}(s)$ coordinatewise for each of the $m$ complex entries of $s$.

For certain distributions $X_\theta$, $S_\theta$ may reduce to the single point 0 or otherwise become degenerate. Our standing assumption will be that $S$ has non-empty interior. Note in this regard that $s \in \text{int} S_\theta$ does not imply $(s, \theta) \in \text{int} S$. The point $0 \in \mathbb{R}^{1 \times m}$ belongs to $S_\theta$ for all $\theta \in R$, although it need not be an interior point of $S_\theta$, for instance when every entry of $X_\theta$ is non-negative with infinite mean. As soon as the interior $\text{int} S_\theta$ is non-empty, $M(s; \theta)$ is analytic as a function of $s \in \text{int} S_\theta$.

### 2.1.2 Gradients and Hessians

Given a row vector argument $s = (s_1 \ s_2 \ \cdots \ s_m) \in \mathbb{R}^{1 \times m}$, we interpret the gradient with respect to $s$ as an $m \times 1$ matrix; applied to a function $f_{\text{row}} : \mathbb{R}^{1 \times m} \to \mathbb{R}^{1 \times k}$ with row-vector values, the result is the $m \times k$ matrix. Thus

$$\nabla s = \begin{pmatrix} \frac{\partial f_1}{\partial s_1} \\ \vdots \\ \frac{\partial f_m}{\partial s_m} \end{pmatrix}, \quad \nabla s f_{\text{row}}(s) = f'_{\text{row}}(s) = \begin{pmatrix} \frac{\partial f_1}{\partial s_1} & \cdots & \frac{\partial f_m}{\partial s_m} \end{pmatrix}, \quad \tag{2.3}$$

and the $i, j$ entry of $f'_{\text{row}}$ is $\frac{\partial f_i}{\partial s_j}$. If instead $x$ is $m \times 1$ and $f = f_{\text{col}} : \mathbb{R}^{m \times 1} \to \mathbb{R}^{k \times 1}$, then $\nabla_x$ has the form of a $1 \times m$ matrix and $\nabla_x f_{\text{col}}(x)$ is the $k \times m$ matrix whose $i, j$ entry is $\frac{\partial f_i}{\partial x_j}$. (Strictly speaking, $\nabla_x$ should operate on $f_{\text{col}}$ from the right if we wish to preserve the usual matrix-shape conventions.) For either of these cases we have

$$\nabla_x^T = (\nabla_x)^T, \quad \nabla_x f = (\nabla_x^T (f^T))^T. \quad \tag{2.4}$$

For scalar-valued functions, $k = 1$, the Hessian matrix of second partial derivatives is

$$f''_{\text{row}}(s) = \nabla_s \nabla_s^T f_{\text{row}}(s) \quad \text{or} \quad f''_{\text{col}}(x) = \nabla_x \nabla_x f_{\text{col}}(x), \quad \tag{2.5}$$

the $m \times m$ symmetric matrix with $i, j$ entry $\frac{\partial^2 f}{\partial s_i \partial s_j}$ or $\frac{\partial^2 f}{\partial x_i \partial x_j}$.

### 2.1.3 Moments and cumulants

With the above conventions, the derivatives $M'(0)$, $M''(0)$ and $K'(0)$, $K''(0)$ give moments and cumulants of $X$:

$$M'(0; \theta) = \mathbb{E}(X_\theta), \quad M''(0; \theta) = \mathbb{E}(X_\theta X_\theta^T),$$

$$K'(0; \theta) = \text{Cov}(X_\theta), \quad K''(0; \theta) = \text{Cov}(X_\theta, X_\theta). \quad \tag{2.6}$$

In particular, $K''(0)$ is positive semi-definite. If $K''(0)$ is singular, then $X$ is supported on a lower-dimensional linear subspace of $\mathbb{R}^{m \times 1}$; in this case we could have discarded one or more entries of $X$ without losing information. We will therefore assume throughout that

$$\det(K''(0)) \neq 0. \quad \tag{2.7}$$

As we will see in Section 3, in this case $K''(s)$ is positive definite and has an interpretation as a non-degenerate covariance matrix, for all $s \in \text{int} S_\theta$, and in particular $K$ is strictly convex as a function of $s$. 

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2.1.4 Multivariate saddlepoint approximation

With these preparations we can state the multivariate saddlepoint approximation. For \( x \in \mathbb{R}^{m \times 1} \), we form the \emph{saddlepoint equation}

\[
K'(\hat{s}; \theta) = x
\]

for \( \hat{s} \in \mathcal{S}_\theta \). The strict convexity of \( K \) implies that if equation (SE) has a solution, then the solution is unique and we call it the \emph{saddlepoint} \( \hat{s} = \hat{s}(\theta; x) \). We write

\[
\mathcal{X}_\theta = \{ x \in \mathbb{R}^{m \times 1} : \exists s \in \mathcal{S}_\theta \text{ solving } K'(s; \theta) = x \}, \quad \mathcal{X} = \{ (x, \theta) : x \in \mathcal{X}_\theta \}.
\]

(2.8)

We will not discuss under what conditions the saddlepoint equation (SE) has a solution; see for instance [12, section 2.1] or [3, Corollary 9.6]. We merely remark that in many common examples, we can solve (SE) for all \( x \) in the interior of the convex hull of the support of \( X \), but that this may fail if, for instance, \( X \) is non-negative with finite mean and infinite variance.

Assuming that the saddlepoint \( \hat{s}(\theta; x) \) solving equation (SE) exists, the \emph{saddlepoint approximation to the likelihood} is

\[
\hat{L}(\theta; x) = \exp\left( K(\hat{s}) - \hat{s}^T x \right) \sqrt{\det(2\pi K''(\hat{s}))},
\]

the multivariate analogue of (1.4). As in (1.6), the saddlepoint MLE \( \hat{\theta}_{\text{MLE}}(x) \) is the value of \( \theta \) that maximises \( \hat{L}(\theta; x) \), if one exists.

We will compare \( \hat{L}(\theta; x) \) and \( \hat{\theta}_{\text{MLE}}(x) \) with the true likelihood \( L(\theta; x) \) and true MLE \( \theta_{\text{MLE}}(x) \). We are assuming that \( X \) has an absolutely continuous distribution, so that the true likelihood \( L(\theta; x) \) should be taken to coincide with the density function for \( X \). Complications can arise if there is ambiguity in the choice of density function – for instance, if the density function has jumps – and later we will impose decay bounds on \( M(s) \) that will imply that \( X \) has a continuous, and therefore essentially unique, density function. Note however that the saddlepoint approximation can be applied whether or not \( X \) has a density function, and indeed we can apply the saddlepoint approximation even when \( X \) has a discrete distribution: see Theorem 5 and Example 6 below.

Throughout the paper we will use the symbol ‘\(^\ast\)’ to indicate saddlepoint approximations, rather than estimators based on observations. Thus \( \theta_{\text{MLE}} \) and \( \hat{\theta}_{\text{MLE}} \) denote two deterministic functions of the formal argument \( x \), whose nature depends on our chosen parametric model. Although we will continue to describe \( x \) as the observed value of \( X \), we will think of \( x \) as the arbitrary input value to the functions \( \theta_{\text{MLE}} \) and \( \hat{\theta}_{\text{MLE}} \), rather than as the result of a random experiment or sampling procedure. When we turn to sampling distributions in Theorem 4, we will introduce further notation to encode the presumed randomness of the observed value.

2.2 The standard asymptotic regime

When we approximate one quantity by another, justification often stems from verifying that the approximation error becomes negligible in some relevant limit. In the case of the saddlepoint approximation, the most common and mathematically tractable limiting framework is to assume that \( X \) is the sum of \( n \) unobserved i.i.d. terms,

\[
X = \sum_{i=1}^n Y^{(i)}, \quad (2.9)
\]
where \( Y^{(1)} , Y^{(2)} , \ldots \) are i.i.d. copies of a random variable \( Y_\theta \) whose distribution does not depend on \( n \). That is, we consider

\[
M(s; \theta) = M_0(s; \theta)^n, \quad K(s; \theta) = nK_0(s; \theta), \quad x = ny, \quad n \to \infty, \quad \text{(SAR)}
\]

where \( M_0 \) and \( K_0 \) are the MGF and CGF corresponding to \( Y_\theta \). Throughout the paper, we will assume the relation \( x = ny \) implicitly, and we think of \( y \) as fixed (or varying within a small neighbourhood) in the limit \( n \to \infty \), so that both \( x \) and \( X \) will be of order \( n \).

We refer to this limiting framework as the standard asymptotic regime for the saddlepoint approximation.

In the standard asymptotic regime, the saddlepoint equation (SE) simplifies to

\[
K'_0(\hat{s}; \theta) = y. \quad \text{(SE_{SAR})}
\]

Write \( Y_\theta \) for the set of \( y \) for which a solution of \((\text{SE}_{\text{SAR}})\) exists, and write \( \hat{s}_0(\theta; y) \) for the function that maps \( y \in Y_\theta \) to the solution of \((\text{SE}_{\text{SAR}})\). Note that the saddlepoint \( \hat{s} \) does not depend on \( n \), and the functions \( \hat{s}(\theta; x) \) and \( \hat{s}_0(\theta; y) \) are related by

\[
\hat{s}(\theta; x) = \hat{s}_0(\theta; y) \quad \text{(2.10)}
\]

when the relations \((\text{SAR})\) hold. We will write \( \hat{s} \) for the common value in \((2.10)\) when the distinction is immaterial. The domains of \( \hat{s} \) and \( \hat{s}_0 \) are related by \( X_\theta = \{ ny : y \in Y_\theta \} \).

In the standard asymptotic regime, the saddlepoint approximation (SPA) becomes

\[
\hat{L}(\theta; x) = \exp \left( \frac{n[K_0(\hat{s}) - \hat{s}y]}{\sqrt{\det(2\pi nK''_0(\hat{s}))}} \right). \quad \text{(SPA_{SAR})}
\]

The basic error estimate for the saddlepoint approximation states that, in the standard asymptotic regime and subject to certain technical assumptions, the relative error in the likelihood is of order \( 1/n \):

\[
\frac{\hat{L}(\theta; x)}{L(\theta; x)} = 1 + O(1/n) \quad \text{as } n \to \infty \quad \text{(2.11)}
\]

for fixed \((y, \theta) \in \mathcal{Y}\). (Note that the \( n \)-dependence of \( L \) and \( \hat{L} \) is omitted from the notation.) See Proposition 15 below for a more precise statement.

In view of the affine invariance of the saddlepoint approximation (see Appendix A), finding the saddlepoint approximation for \( X \) is equivalent to finding the saddlepoint approximation for \( \overline{Y} = \frac{1}{n}X \), the sample mean of the i.i.d. values \( Y^{(1)}, \ldots, Y^{(n)} \) from \((2.9)\). It can be helpful to interpret the value \( y = x/n \) from equation \((\text{SAR})\) as the observed value of this sample mean. However, we will consider \( X \) rather than \( \overline{Y} \), not least because the saddlepoint for \( X \) does not depend on \( n \).

**Remark.** The standard asymptotic regime supposes that the observed value \( X \) is the sum of \( n \) unobserved i.i.d. terms. That is, we have only a single observation, \( X = x \), rather than \( n \) observations of the summands \( Y^{(1)}, \ldots, Y^{(n)} \). For this reason, the parameter \( n \) should not be interpreted as a sample size. On the contrary, if we observe \( k \) i.i.d. samples \( X^{(1)}, \ldots, X^{(k)} \) from the distribution \( X_\theta \), so that the observed data forms a vector of dimension \( km \), a quite different asymptotic result applies when \( k \to \infty \); see the discussion in Section 2.5.5.
2.3 Main results

We prove a general asymptotic error bound for the derivative of the true and saddlepoint log-likelihoods; the resulting error bound for the corresponding MLEs, and distributional limits for the corresponding posterior and sampling distributions. The latter results include the asymptotic normality that applies when using the true likelihood in the limiting framework (SAR), which may be of independent interest.

Because we wish to understand the true and approximate likelihoods as functions of $\theta$, our central objects of study will be $\nabla_\theta \log L$ and $\nabla_\theta \log \hat{L}$ rather than $L$ and $\hat{L}$. As we will see in Section 3.1, $L$ and its derivatives can be expressed as integrals involving $M_0(s + i\varphi)$ and its derivatives, where $s$ is fixed and $\varphi$ is integrated over $\mathbb{R}^{1 \times m}$. To ensure that these integrals converge, we make the following technical assumptions on the growth or decay of $M_0$ and its derivatives:

there is a continuous function $\delta$: $\text{int } S \to (0, \infty)$ such that

$$\left| \frac{M_0(s + i\varphi; \theta)}{M_0(s; \theta)} \right| \leq (1 + \delta(s, \theta)|\varphi|^2)^{-\delta(s, \theta)} \quad \text{for all } \varphi \in \mathbb{R}^{1 \times m}, (s, \theta) \in \text{int } S,$$

(2.12)

there is a continuous function $\gamma$: $\text{int } S \to (0, \infty)$ such that

$$\left| \frac{\partial^{k+\ell} M_0}{\partial \theta_1 \cdots \partial \theta_k \partial s_{j_1} \cdots \partial s_{j_\ell}} (s + i\varphi; \theta) \right| \leq \gamma(s, \theta)(1 + |\varphi|)^{\gamma(s, \theta)}$$

for all $\varphi \in \mathbb{R}^{1 \times m}$ and $(s, \theta) \in \text{int } S$,

for $k \in \{0, 1\}$, $1 \leq k + \ell \leq 6$ and for $k = 2$, $0 \leq \ell \leq 2$,

and with each of these partial derivatives continuous in all its variables.

Our results for the saddlepoint MLE are based on the following general bound on the difference between the gradients of $\log L$ and $\log \hat{L}$.

Theorem 1 (Gradient error bound). If (SAR), (2.7) and (2.12)–(2.13) hold and $(y, \theta) \in \text{int } \mathcal{Y}$, then

$$\nabla_\theta \log \hat{L}(\theta; x) = \nabla_\theta \log L(\theta; x) + O(1/n) \quad \text{as } n \to \infty.$$

(2.14)

If $(y, \theta)$ is restricted to a compact subset of $\text{int } \mathcal{Y}$, the bound in the term $O(1/n)$ is uniform.

We obtain accuracy bounds for the MLE by applying the gradient error bound from Theorem 1 (or rather, its more precise analogues from Section 4.2) in the neighbourhood of a local maximizer. In the next result, we suppose that we can find a parameter $\theta_0$ that is a local maximizer, not for the full saddlepoint approximation from (SPA$\text{SAR}$), but for the function

$$\theta \mapsto K_0(s_0(\theta; y); \theta) - s_0(\theta; y)y$$

(2.15)

that appears in the leading-order exponential factor of (SPA$\text{SAR}$). Under the assumption that the critical point $\theta_0$ is non-degenerate, we show that both the true MLE and the saddlepoint MLE have local maximizers near $\theta_0$, and give estimates for the distances between these two local maximizers. As we will see later, the expressions in (2.17)–(2.18) below are the gradient and Hessian, respectively, of the function in (2.15); see Section 4.1 and Appendix B.

Theorem 2 (MLE error bound). Let $(s_0, \theta_0) \in \text{int } \mathcal{S}$ and $y_0 \in \text{int } \mathcal{Y}_{\theta_0}$ be related by

$$y_0 = K_0'(s_0; \theta_0),$$

(2.16)
and suppose that (SAR), (2.7) and (2.12)–(2.13) hold. Suppose in addition that
\[ \nabla_{\theta} K_0(s_0; \theta_0) = 0 \]
and that
\[ H = \nabla_{\theta}^2 \nabla_{\theta} K_0(s_0; \theta_0) - (\nabla_s \nabla_{\theta} K_0(s_0; \theta_0))^T K_0''(s_0; \theta_0)^{-1} (\nabla_s \nabla_{\theta} K_0(s_0; \theta_0)) \]
is negative definite.

Then there exist \( n_0 \in \mathbb{N} \) and neighbourhoods \( U \subset R \) of \( \theta_0 \) and \( V \subset \mathbb{R}^{m \times 1} \) of \( y_0 \) such that, for all \( n \geq n_0 \) and \( y \in V \), the functions \( \theta \mapsto \hat{L}(\theta; x) \) and \( \theta \mapsto L(\theta; x) \) have unique local maximizers in \( U \). Moreover, writing these local maximizers as \( \hat{\theta}_{\text{MLE in } U}(x) \) and \( \theta_{\text{MLE in } U}(x) \),
\[ \left| \hat{\theta}_{\text{MLE in } U}(x) - \theta_{\text{MLE in } U}(x) \right| = O(1/n^2) \quad \text{as } n \to \infty \]
uniformly over \( n \geq n_0 \), \( y \in V \).

We next compare \( L \) and \( \hat{L} \) by considering their shape in a neighbourhood of the maximum. In a Bayesian framework, let the parameter \( \Theta \) be drawn according to a prior \( \pi_\Theta \) on \( R \). For a given observed value \( x \), we will consider the posterior distribution \( \pi_{\Theta | U,x} \) on a neighbourhood \( U \subset R \) with \( \pi_{\Theta}(U) > 0 \), defined by the Radon-Nikodym derivative
\[ \frac{d\pi_{\Theta | U,x}}{d\pi_{\Theta}}(\theta) = \frac{\hat{L}(\theta; x) 1_{\{\theta \in U\}}}{C}, \quad C = C_{U,x} = \int_U L(\theta; x) d\pi_{\Theta}(\theta). \]

We construct the saddlepoint posterior distribution on \( U \), \( \hat{\pi}_{\Theta | U,x} \), by replacing \( L \) by \( \hat{L} \):
\[ \frac{d\hat{\pi}_{\Theta | U,x}}{d\pi_{\Theta}}(\theta) = \frac{\hat{L}(\theta; x) 1_{\{\theta \in U\}}}{\hat{C}}, \quad \hat{C} = \int_U \hat{L}(\theta; x) d\pi_{\Theta}(\theta). \]

**Theorem 3 (Posterior distributions).** Let \((s_0, \theta_0) \in \text{int } S\) and \( y_0 \in \mathcal{Y}_{\theta_0} \) be related as in (2.16), and suppose that (SAR), (2.7), (2.12)–(2.13) and (2.17)–(2.18) hold. Suppose also that the prior distribution \( \pi_\Theta \) has a probability density function that is continuous and positive at \( \theta_0 \). Fix \( y = y_0, x = ny_0 \). Then there exists a neighbourhood \( U \subset R \) of \( \theta_0 \) such that
\[ \text{under } \pi_{\Theta | U,x} \text{ or } \hat{\pi}_{\Theta | U,x}, \quad \sqrt{n} (\Theta - \theta_0) \overset{d}{\to} \mathcal{N}(0, -H^{-1}) \quad \text{as } n \to \infty, \]
where \( H \) is the negative definite matrix from (2.18).

The proof of Theorem 3 will follow from a stronger statement, Proposition 23, that removes the assumption \( y = y_0 \).

Theorems 2 and 3 concern the deterministic functions that map an observed value \( x \) to the corresponding MLE or posterior distribution, via either the true likelihood or the saddlepoint approximation. In this description, the observed value \( x \) has been treated as deterministic, separate from any consideration of the random process that might have generated this observation. In particular, Theorems 1–3 do not make any statement about the sampling distribution of an estimator.

The next theorem describes the sampling distribution when the observation is itself a random variable \( \xi_n \). Since the model assumes that \( X \) is a sum of \( n \) i.i.d. summands \( Y^{(i)} \), as in (2.9), it is natural to consider the case
\[ \xi_n = \sum_{i=1}^{n} \zeta^{(i)} \quad \text{where } \zeta^{(1)}, \zeta^{(2)}, \ldots \text{ are i.i.d. with finite second moments.} \]
As with $X$, we consider $\xi_n$ as a column vector with values in $\mathbb{R}^{m \times 1}$. Then (2.23) implies
\[
\frac{\xi_n - ny_0}{\sqrt{n}} \xrightarrow{d} \mathcal{N}(0, \Sigma)
\] (2.24)
where $y_0 \in \mathbb{R}^{m \times 1}$ corresponds to $\mathbb{E}(\zeta^{(1)})$ and the positive semi-definite matrix $\Sigma \in \mathbb{R}^{m \times m}$ corresponds to $\text{Cov}(\zeta^{(1)}, \zeta^{(1)})$. In Theorem 4, part (a) applies to the mis-specified case where the distributions of $\zeta^{(1)}$ and $\xi_n$ need not equal those of $Y_0$ and $X_0$, respectively, for any value of $\theta$. Part (b) applies to the well-specified case where $\zeta^{(1)}$ and $\xi_n$ have the same mean vectors and covariance matrices as $Y_{\theta_0}$ and $X_{\theta_0}$, respectively, in which case some simplification occurs; see also the remarks in Section 2.5.4 below. Note however that Theorem 4 does not require $\xi_n$ to have the form (2.23), provided that (2.24) holds.

**Theorem 4** (Sampling distributions). Let $(s_0, \theta_0) \in \text{int } \mathcal{S}$ and $y_0 \in \text{int } \mathcal{Y}_{\theta_0}$ be related as in (2.16), suppose that (2.7), (2.12)–(2.13), (2.17) and (2.18) hold, and suppose that (2.24) holds for some positive semi-definite matrix $\Sigma \in \mathbb{R}^{m \times m}$. Let $U$ be the neighbourhood of $\theta_0$ given by Theorem 2. Then:

(a) The joint sampling distribution of the true and saddlepoint MLEs satisfies
\[
\left( \sqrt{n} \left( \theta_{\text{MLE in } U} (\xi_n) - \theta_0 \right), \sqrt{n} \left( \hat{\theta}_{\text{MLE in } U} (\xi_n) - \theta_0 \right) \right) \xrightarrow{d} (Z, Z) \quad \text{as } n \to \infty, \quad (2.25)
\]
with
\[
Z \sim \mathcal{N} \left( 0, H^{-1} B^T A^{-1} \Sigma A^{-1} B H^{-1} \right) \quad (2.26)
\]
where we have abbreviated $A = K''(s_0; \theta_0)$, $B = \nabla_{s} \nabla_{\theta} K_0(s_0; \theta_0)$, and $H$ is the negative definite matrix from (2.18).

(b) If in addition $y_0 = K'(0; \theta_0)$ and $\Sigma = K''(0; \theta_0)$ then the limiting distribution has
\[
Z \sim \mathcal{N} \left( 0, -H^{-1} \right). \quad (2.27)
\]

Finally all of these results apply to integer-valued random variables – although, as we shall discuss in Section 2.5.2, it would be natural to make different and more flexible assumptions in the integer-valued case.

**Theorem 5.** Let $X_0$ have values in $\mathbb{Z}^{m \times 1}$ and set $L(\theta; x) = \mathbb{P}(X_0 = x)$, with the restriction $x \in \mathbb{Z}^{m \times 1}$. Then the results of Theorems 1–4 hold, with the assumption (2.12) replaced by the assumption that $|M_0(s + i \varphi; \theta)| < M_0(s; \theta)$ for all $(s, \theta) \in \text{int } \mathcal{S}$ and $\varphi \in (-\pi, \pi)^{1 \times m} \setminus \{0\}$.

A key conclusion from our results is that the approximation error in using the saddlepoint MLE in place of the true MLE is negligible, in the limit $n \to \infty$ as in (SAR), compared to the underlying inferential uncertainty. Namely, according to Theorem 2, the difference between the true and saddlepoint MLEs is of order $1/n^2$. Asymptotically, this approximation error is much smaller than the spatial scale $1/\sqrt{n}$ corresponding to either sampling variability of the MLE (in the frequentist setup of Theorem 4) or posterior uncertainty of the parameter (in the Bayesian setup of Theorem 3). At least to the extent that the assumptions of the standard asymptotic regime apply in a given application, the saddlepoint likelihood and saddlepoint MLE are therefore appropriate as readily-calculated substitutes for the true likelihood and MLE.
2.4 Examples

In this section, we show how the saddlepoint MLE and the results of this paper apply for certain specified distributions, and for a range of applications in the literature. As we shall see, most examples from the literature fall into the standard asymptotic regime either exactly, or with moderate modifications.

Example 6 (Poisson distribution). Let \( X_\theta \sim \text{Poisson}(\theta) \), corresponding to

\[
K(s) = \theta(e^s - 1), \quad \hat{s} = \log(\frac{x}{\theta}), \quad \hat{f}(x) = \exp\left(\frac{\theta(x/\theta - 1) - x \log(x/\theta)}{\sqrt{2\pi\theta(x/\theta)}}\right) = e^{-\theta e^x} \frac{(e/x)^x}{\sqrt{2\pi x}}.
\]

Note that \( \hat{f}(x) \) is well-defined even though \( X \) does not have a density, and \( \hat{f}(x) \) is a reasonable approximation to \( \mathbb{P}(X = x) \) for \( x \in \mathbb{N} \), corresponding to Stirling’s approximation to \( x! \) with relative error of order \( 1/x \). Note also that as an approximation to the likelihood, the saddlepoint approximation is essentially exact for all \( x > 0 \) since it has the form \( c(x) \mathbb{P}(X_\theta = x) \) where \( c(x) \) depends on \( x \) but not \( \theta \). In particular, the saddlepoint MLE is exact.

If instead we write \( Y_{\theta'} \sim \text{Poisson}(\theta') \) and \( X = \sum_{i=1}^n Y_{\theta'}^{(i)} \) in the setup of (SAR), then \( X \sim \text{Poisson}(n\theta') \). This amounts to a reparametrisation \( \theta = n\theta' \), and if we expect an observation \( x \) of order \( n \) we can set \( x = ny \) with \( y > 0 \) of constant order, as in (SAR).

Indeed the relative error in the likelihood, for an observed value on the scale \( x = ny \), is of order \( 1/n \) as suggested by (2.11).

The phenomenon of Example 6 holds more generally:

Example 7 (Exponential family). Let \( X \) be a sufficient statistic for an exponential family of distributions with natural parameter \( \eta \in \mathbb{R}^{1 \times m} \), with

\[
f_X(x; \theta = \eta^T) = h(x) \exp(\eta x - \rho(\eta)), \quad K_X(s; \eta^T) = \rho(\eta + s) - \rho(\eta)
\]

for scalar functions \( h, \rho \) with \( \rho \) convex. The saddlepoint equation (SPA) reduces to

\[
\rho'(\eta + \hat{s}) = x.
\]

In particular, the quantity \( \hat{\eta} = \eta + \hat{s} \) depends on \( x \) alone and is fixed as a function of \( \eta \).

The saddlepoint approximation can be written as

\[
\hat{f}(x; \eta^T) = \frac{\exp(\rho(\hat{\eta}) - \hat{\eta}x)}{\sqrt{\det(2\pi \rho''(\hat{\eta}))}} \exp(\eta x - \rho(\eta)).
\]

The first factor need not coincide with \( h(x) \), so the saddlepoint approximation need not be exact, but because the first factor depends on \( x \) only, the saddlepoint MLE is exact for an exponential family provided that the saddlepoint approximation itself is well-defined. Indeed, the MLE is precisely the quantity \( \hat{\eta} = \eta + \hat{s} \) that solves \( \rho'(\hat{\eta}) = x \), which we already find in the course of computing the saddlepoint.

Example 8. Let \( Z \) have the Gamma distribution with shape parameter \( \alpha \) and rate parameter \( r \). As is well known, the Gamma family is an exponential family of distributions. However, the details of the saddlepoint approximation, and the way in which the conclusions of Example 7 apply to MLEs, vary depending on the exact choice of \( X \).
If we set $Y_1 = Z$, then $X_1$ will have the Gamma($n\alpha, r$) distribution and we find

$$K_{Y_1}(s) = \alpha \log \frac{r}{r-s}, \quad \hat{s}_1 = r - \frac{\alpha}{y} \quad \hat{f}_1(x) = r^{na}x^{na-1}e^{-rx} \frac{e^{na}}{(na)^{na-1/2}2\pi}. \quad (2.32)$$

As a function of $r$, $\hat{f}_1(x)$ is a constant multiple of the true density, so using $\hat{f}_1$ to approximate the MLE for $r$ will be exact. However, the last factor in $\hat{f}_1(x)$ is not a constant multiple of $1/\Gamma(n\alpha)$ – in fact it is the reciprocal of Stirling’s approximation to $\Gamma(n\alpha)$ – so using $\hat{f}_1$ to approximate the MLE for $\alpha$ will not be exact. In the framework of Example 7, this corresponds to the observation that $X_1$ (or $Y_1$) is the sufficient statistic for the sub-family in which $r$ varies but $\alpha$ is fixed.

If we set $Y_2 = \log Z$, we can still compute the MGF and CGF:

$$M_{Y_2}(t) = r^{-\gamma}\frac{\Gamma(\alpha + t)}{\Gamma(\alpha)}, \quad K_{Y_2}(t) = \psi(\alpha + t) - \log r, \quad (2.33)$$

where $\psi(z) = \Gamma'(z)/\Gamma(z)$ denotes the digamma function. The saddlepoint equation has no elementary solution but can be solved numerically. Now $Y_2$ is the sufficient statistic for the sub-family in which $\alpha$ varies and $r$ is fixed, so using $\hat{f}_2$ to find the MLE for $\alpha$ will be exact.

Finally we can set $Y_3 = (Z, \log Z)^T$, the bivariate sufficient statistic for the entire Gamma exponential family:

$$M_{Y_3}(s, t) = \frac{r^\alpha}{(r-s)^{\alpha+t}} \frac{\Gamma(\alpha + t)}{\Gamma(\alpha)}, \quad \frac{\partial K_{Y_3}}{\partial s} = \frac{\alpha + t}{r-s}, \quad \frac{\partial K_{Y_3}}{\partial t} = \psi(\alpha + t) - \log(r-s). \quad (2.34)$$

The saddlepoint equation does not have an elementary solution, but the quantities $\hat{\alpha} = \hat{\alpha}_3 = \alpha + \hat{t}_3$ and $\hat{r} = \hat{r}_3 = r - \hat{s}_3$ will depend only on the observed value $x_3$ and not on $\alpha$ or $r$. Specifically, if we write $x_3 = ny_3$ with $y_3 = (\bar{z}, \bar{\ell})^T$, then $\hat{\alpha}, \hat{r}, \hat{f}_3$ are determined by

$$\psi(\hat{\alpha}) - \log \hat{\alpha} = \bar{\ell} - \log \bar{z}, \quad \hat{r} = \frac{\hat{\alpha}}{\bar{z}}, \quad \hat{f}_3(x_3) = \left(\frac{r^\alpha e^{\alpha \bar{\ell} - \bar{r}x}}{\Gamma(\alpha)}\right)^n \frac{\hat{\alpha} [\Gamma(\hat{\alpha})e^{\hat{\alpha}(1-\Psi(\hat{\alpha}))}]^n}{2\pi n \sqrt{\hat{\alpha}\psi(\hat{\alpha}) - 1}}. \quad (2.35)$$

Consulting for instance [10, equation 8.361.3], we see that the function $\alpha \mapsto \psi(\alpha) - \log \alpha$ is strictly increasing and maps $(0, \infty)$ to $(-\infty, 0)$. So (2.35) will have a solution if and only if $\bar{z} > 0$ and $\bar{\ell} < \log \bar{z}$.

In practice, this means that the saddlepoint approximation for $X_3$ can only be applied when $n \geq 2$. For the case $n = 1$, the values of $Y_3$ will lie on the curve $\bar{\ell} = \log \bar{z}$ where $\hat{\alpha}$ is undefined, and $Y_3$ does not have a density; likewise if we take $\bar{z} \searrow e^{\ell}$, we can verify that $\hat{\alpha} \to \infty$ and $\hat{f} \to \infty$. On the other hand, as soon as $n \geq 2$, $X_3$ is supported in the region where $\bar{\ell} < \log \bar{z}$ (this is Jensen’s inequality applied to the summands $Y_3^{(1)}, \ldots, Y_3^{(n)}$) and $f_3$ is finite there. As in Example 7, as soon as $n \geq 2$, using $f_3$ to find the MLEs for both $r$ and $\alpha$ will be exact.

**Example 9 (Linear mapping).** Let $X = AU$, where $A \in \mathbb{R}^{m \times k}$ is a fixed matrix and $U = U_\theta \in \mathbb{R}^{k \times 1}$ is an unobserved random vector whose moment generating function is known. We are interested in the case $k > m$, with $A$ of maximal rank $m$, so that $X$ has non-singular covariance matrix if $U$ does. Since $A$ is not invertible, observing $X$ does not allow us to identify the value of $U$, and a straightforward approach to computing the likelihood for $X$ requires integrating over a $(k - m)$-dimensional subspace of $U$ values
compatible with a given $X$ value. However, the moment generating function of $X$ can be readily calculated by $M_X(s) = M_U(sA)$, making the saddlepoint approximation an attractive alternative that avoids lengthy approximate integration.

A common case is that the entries of $U$ are independent, so that columns of $A$ with several non-zero entries induce dependencies between the entries of $X$. In the context of our results, assuming that $X$ is the sum of $n$ i.i.d. terms, as in (SAR), amounts to the assumption that $U$ is itself the sum of $n$ i.i.d. terms.

**Example 10** (Branching processes). Davison, Hautphenne & Kraus [8] estimate the parameters of a birth-death process observed at discrete observation times, using a saddlepoint approximation to the transition probabilities. In our notation, $X$ is the population size at a given observation time.

By the branching process property, $X$ is modelled as the sum of $n$ i.i.d. terms, where $n$ is the population size at the previous observation time. Thus the problem falls into the standard asymptotic regime considered in (SAR), with $Y$ corresponding to the offspring distribution from a single individual. In practice, multiple observations are made over time, and the observed population size $x_i$ at time step $i$ also plays the role of the number of summands $n_{i+1}$ at the following step. To match the setup of (SAR), write the vector of observations as $(x_i) = n(y_i)$. To the extent that we can make $n$ large while keeping the entries $y_i$ bounded away from 0 and $\infty$, the conclusions of Theorem 5 will apply. (A slightly different question, which is beyond the scope of this paper, is to understand the asymptotic accuracy when some, but not all, of the entries $x_i$ become large.)

It is noteworthy that the applicable value of $n$ is determined by the data (here, the sizes of the population at various times) rather than by the data-collection procedure.

**Example 11** (Capture-recapture and table data). Zhang, Bravington & Fewster [21] consider count data of the form $X = AU$ as in Example 9, with applications to capture-recapture in ecological and human contexts. Here the vector $X$ contains counts of various observed capture histories after including the corrupting effects of misidentification. The deterministic matrix $A$ encodes how a true capture history (counted by $U$) may be counted more than once in $X$. Note that a capture-recapture experiment naturally produces only a single observation, the vector of counts of different capture histories across all capture-recapture occasions, rather than a sample of many i.i.d. observations.

The vector $U$ is modelled as a Multinomial distribution, with $N$, the unknown overall population size, specifying the number of trials. Thus $U$ is the sum of $N$ i.i.d. vectors encoding the true capture histories, so that $X$ is also the sum of $N$ i.i.d. vectors and the standard asymptotic regime (SAR) applies with $n = N$. Here the value of $N$ is unknown – indeed it is the main parameter whose value is to be inferred from data. The inferential setup of Theorems 1–5 does not directly apply, because the unknown parameter $N$ is discrete rather than continuous. Nevertheless, our results suggest that inference on $N$ will have little approximation error, particularly if $N$ is large, and this is in line with the empirical findings in [21]. (In practice, some adaptation is necessary because $X$ typically includes some zero counts, which cause the saddlepoint approximation to fail if not accounted for.)

We can adapt the model from [21] to the inferential setup of Theorems 1–5 by recasting the discrete parameter $N$ as a random variable with a continuous parameter. If we model $N \sim \text{Poisson}(\lambda)$, as is commonly assumed in capture-recapture models, then the entries of $U$ will have independent Poisson distributions with parameters proportional to $\lambda$. As in Example 6, if we expect observed counts of order $n$, we should substitute $\lambda = n\lambda'$. 
Then (SAR) and the framework of Theorems 1–5 apply, and state that the relative error for approximating $\lambda'_{\text{MLE}}$ by $\hat{\lambda}'_{\text{MLE}}$, and therefore also $\lambda_{\text{MLE}}$ by $\hat{\lambda}_{\text{MLE}}$, will be of order $1/n^2$ in the limit $n \to \infty$.

**Example 12** (INAR($p$) model). Pedeli, Davison & Fokianos [15] fit time series data to an integer-valued autoregressive process given by $X_{i+1} \sim \text{Binomial}(X_i, p) + \epsilon_i$. That is, the process undergoes Binomial thinning at each step, counteracted by i.i.d. integer-valued “innovations” $\epsilon_i$. As in Example 10, the saddlepoint approximation is applied to the one-step transition probabilities, $X = X_{i+1}$ with $X_i = x_i$ fixed. This model does not quite fall into the standard asymptotic regime because of the innovations $\epsilon_i$, but if these were absent then the setup of (SAR) would apply with $n = x_i$ and $Y$ having the Bernoulli($p$) distribution. The results in this paper therefore provide a starting point for the analysis of this more elaborate scenario, and it is reasonable to expect similar results to apply.

As in Example 10, the values of $n$ are determined by the time series data values that are being fit to the model, not the sample size.

**Example 13** (Saddlepoint approximations for diffusions). A"ıt-Sahalia & Yu [1] apply saddlepoint techniques to approximate transition probabilities for diffusions, taking $X$ to be the location of the diffusion process after a short time interval $t$. The setup of (SAR) does not apply; instead, $X$ becomes approximately normal in the limit $t \to 0$, and $t$ plays a role analogous to that of the quantity $1/n$.

### 2.5 Discussion

**2.5.1 Application and scope of the results**

The scope for applying saddlepoint methods is limited to situations where we know the moment generating function $M(s)$ exactly (or can calculate it to high precision on a computer). We caution that substituting an approximation for $M(s)$ or $K(s)$ (for instance, a Taylor approximation based on finitely many moments or cumulants) may give disappointing results, as the saddlepoint approximation relies on knowing the exact values of $K(\hat{s}), K'(\hat{s})$ even when $\hat{s}$ is far from 0. A special case that skips some of the possible pitfalls is to replace $K(s)$ by its Taylor series of order 2: this amounts to a traditional normal approximation based on the mean and variance of the underlying distribution (see also [8, Section 5]).

Even with these restrictions, the saddlepoint approximation can be applied in a variety of examples, as in Section 2.4, and gives a robust approximation to the likelihood and MLE. Moreover, it may be simple to compute even when the true likelihood is intractable. The results in this paper show that the saddlepoint MLE offers a high degree of asymptotic accuracy. Most notably, the MLE carries an intrinsic spatial scale of order $1/\sqrt{n}$, and by comparison the saddlepoint approximation error, of order $1/n^2$, is negligible in the limit $n \to \infty$.

This encouraging asymptotic result should, like many limiting statements, be interpreted with some caution in practice. In a typical application, we consider only one value of $n$ rather than a sequence tending to infinity. For instance, in practice, rather than verifying that the Hessian from (2.18) is non-singular at a specified base point $\theta_0$, we should enquire whether the Hessian is nearly singular in a reasonable neighbourhood of the computed saddlepoint MLE $\hat{\theta}_{\text{MLE}}(x)$.

Furthermore, the saddlepoint approximation can be used regardless of whether the model falls into the standard asymptotic regime described here. Indeed, we have followed
Butler in thinking of \((\text{SPA}_{\text{SAR}})\) as the special case of \((\text{SPA})\) where \(X\) is a sum of \(n\) i.i.d. terms, rather than thinking of \((\text{SPA})\) as the special case of \((\text{SPA}_{\text{SAR}})\) where \(n = 1\); see \([5, \text{section 2.2.2}]\). Even when the model directly assumes a sum of \(n\) i.i.d. terms, the value of \(n\) is in many cases determined by the values of the data, as in Examples 10–12, rather than the size of the data set. (Here we reiterate, as remarked in Section 2.2, that \(n\) does not represent a sample size; see also Section 2.5.5 below.) Thus we may not be able to make \(n\) large, whereas we can often envisage increasing the sample size in a traditional large-sample limit.

Finally, we note that our results concern local maxima and local neighbourhoods in parameter space. The true likelihood \(L(\theta; x)\) may have a complicated structure as a function of \(\theta\), with multiple local maxima, and the saddlepoint approximation cannot do better than faithfully replicating this complicated structure. Moreover, the saddlepoint approximation might have greater error in distant parts of parameter space, so that the saddlepoint MLE might fail to exist globally even if the true likelihood has a global maximum. This possibility does not usually arise in practice but seems difficult to rule out a priori. We note however that, because our results hold uniformly in a neighbourhood of a given point \(y_0\), they apply in situations such as the setup of \((2.23)\): the observed sample means \(\frac{1}{n}\xi_n\) are in principle supported on \(\mathbb{R}^m\) but will lie in a neighbourhood of \(y_0 = E(\zeta(1))\) in the limit \(n \to \infty\).

### 2.5.2 The integer-valued case

On the face of it, the discrete Theorem 5 parallels quite closely the continuous Theorems 1–4: the conclusions are identical, and the hypotheses are quite similar. There is however an important contextual difference: in the discrete case, the restriction to the interiors of \(S\) and \(Y\) excludes values of interest. For instance, suppose \(X\) represents count data, \(X \in \mathbb{Z}^{m \times 1}\). If we observe a count of 0 (or an observed vector including one or more zero counts) then we will be unable to find the saddlepoint \(\hat{s}\). Even if we circumvent this issue by interpreting \(\hat{s}\) as the limit \(s \to -\infty\), the resulting saddlepoint approximation will still diverge, and no MLE can be computed.

This problem arises in part because integer-valued random variables are more naturally studied in terms of their probability generating function \(G(z) = E(z^X)\) rather than \(M(s)\), corresponding to the change of variables \(z = e^s\). Thus the assumption on \(M_0\) from Theorem 5 is expressed in terms of \(G\) by saying that, restricted to \(\{z: |z| = r_i, i = 1, \ldots, m\}\), the function \(|G(z)|\) has a unique maximum at \(z = (r_1 \cdots r_m)\). Likewise, the assumption \((2.13)\) simplifies: \(M_0(s + i\varphi; \theta)\) and its derivatives are periodic as functions of \(\varphi\), so it suffices to verify that they are continuous.

Furthermore, as we shall discuss in Section 3.1, the saddlepoint approximation is fundamentally a (normal) density approximation, and it can be problematic when applied as an approximation for a probability mass function. It is the author’s intention to return to these questions in future research.

### 2.5.3 Heuristic for the true MLE and saddlepoint MLE

We can give a heuristic argument for how the size of the gradient error from Theorem 1 leads to the size of the MLE error in Theorem 2. Namely, fix \(x = ny_0\) and assume as a simplification that

- the function \(\theta \mapsto K_0(\hat{s}_0(\theta; y_0); \theta) - \hat{s}_0(\theta; y_0)y_0\) from \((2.15)\) – which by \((2.17)-(2.18)\)
has a non-degenerate local maximum at $\theta = \theta_0$ — is purely quadratic around its maximum value, say $\theta \mapsto a + \frac{1}{2}(\theta - \theta_0)^T H(\theta - \theta_0)$ where $H$ is negative definite;

- the function $\theta \mapsto -\frac{1}{2} \log \det \mathcal{K}''(\hat{s}(\theta; y_0); \theta)$ is purely affine, say $\theta \mapsto b + u(\theta - \theta_0)$ for some fixed $u \in \mathbb{R}^{1 \times p}$; and

- the difference $\nabla_\theta \log \hat{L}(\theta; x) - \nabla_\theta \log L(\theta; x)$ from Theorem 1 has the form $\frac{1}{n} v$ for some fixed $v \in \mathbb{R}^{1 \times p}$.

Under these assumptions

$$\log \hat{L}(\theta; x) = na + \frac{1}{2} n(\theta - \theta_0)^T H(\theta - \theta_0) - \frac{m}{2} \log(2\pi n) + b + u(\theta - \theta_0)$$  \hspace{1cm} (2.36)

and we can complete the square to find

$$\log \hat{L}(\theta; x) = \frac{1}{2} n (\theta - \theta_0 + \frac{1}{n} H^{-1} u^T)^T H \left( \theta - \theta_0 + \frac{1}{n} H^{-1} u^T \right) - \frac{1}{2n} u H^{-1} u^T + na - \frac{m}{2} \log(2\pi n) + b.$$  \hspace{1cm} (2.37)

Thus the saddlepoint MLE comes to

$$\hat{\theta}_{\text{MLE}}(x) = \theta_0 - \frac{1}{n} H^{-1} u^T.$$

(2.38)

For the true likelihood, define the constants $c_n = \log \hat{L}(\theta_0; x) - \log L(\theta_0; x)$. Then

$$\log L(\theta; x) = na + \frac{1}{2} n(\theta - \theta_0)^T H(\theta - \theta_0) - \frac{m}{2} \log(2\pi n) + b + u(\theta - \theta_0) - c_n - \frac{1}{n} v(\theta - \theta_0).$$  \hspace{1cm} (2.39)

Comparing (2.39) with (2.36), we see that changing from $\hat{L}$ to $L$ amounts to replacing $u$ by $u - \frac{1}{n} v$ and subtracting a constant term $c_n$. We can again complete the square to find

$$\log L(\theta; x) = \frac{1}{2} n \left( \theta - \theta_0 + \frac{1}{n} H^{-1} u^T - \frac{1}{n} H^{-1} v^T \right)^T H \left( \theta - \theta_0 + \frac{1}{n} H^{-1} u^T - \frac{1}{n} H^{-1} v^T \right) - \frac{1}{2n} (u - \frac{1}{n} v) H^{-1} (u - \frac{1}{n} v)^T + na - \frac{m}{2} \log(2\pi n) + b - c_n$$

leading to

$$\theta_{\text{MLE}}(x) = \theta_0 - \frac{1}{n} H^{-1} u^T + \frac{1}{n} H^{-1} v^T,$$

(2.40)

with an extra term of order $1/n^2$ in accordance with Theorem 2.

In this heuristic, note that the size of $c_n$ (the error term in the log-likelihood approximation at $\theta = \theta_0$) was irrelevant to the size of the MLE error. So indeed was the term $-\frac{m}{2} \log(2\pi n)$ in $\log \hat{L}$. In fact, even if we drop all terms arising from the factor $(\det(2\pi \mathcal{K}''(\hat{s})))^{-1/2}$ in the saddlepoint approximation $\hat{L}$, the heuristic above suggests that the resulting MLE approximation would still be within $O(1/n)$ of the true MLE. This intuition is correct: see Proposition 14 below.

### 2.5.4 The well-specified case

In Theorems 2–5, some simplification occurs if

$$y_0 = \mathbb{E}(Y_{\theta_0}),$$

(2.42)

i.e., if the observed sample mean matches with the model mean for some parameter value. In this case we might say that the model is “well-specified at the level of the mean.”
If (2.42) holds, we see that $s_0 = 0$ is the solution of the saddlepoint equation $K'_0(s_0) = y_0$. Since $K_0(0; \theta) = 0$ for all $\theta$, it follows that

$$
\nabla_\theta K_0(0; \theta_0) = 0, \quad \nabla_\theta^T \nabla_\theta K_0(0; \theta_0) = 0.
$$

(2.43)

Thus the condition (2.17) holds automatically, and the matrix $H$ from (2.18) simplifies to

$$
H = -(\nabla_s \nabla_\theta K_0(0; \theta_0))^{1/2} K''_0(0; \theta_0)^{-1/2}(\nabla_s \nabla_\theta K_0(0; \theta_0)).
$$

(2.44)
The matrix $K''_0(0; \theta_0)$ is already positive definite by assumption, see (2.7), so the condition (2.18) is equivalent to assuming that

$$
\nabla_s \nabla_\theta K_0(0; \theta_0) \text{ has rank } p.
$$

(2.45)

We can recognise the $m \times p$ matrix $\nabla_s \nabla_\theta K_0(0; \theta_0)$ as the gradient of the mapping

$$
\theta \mapsto \mathbb{E}(Y_\theta)
$$

(2.46)

(evaluated at $\theta_0$) and the condition (2.18)/(2.45) is equivalent to saying that the linear approximation (at $\theta_0$) to the mapping $\theta \mapsto \mathbb{E}(Y_\theta)$ is one-to-one. We might describe the condition (2.18)/(2.45) as saying that the model is “identifiable at the level of the mean.”

Heuristically, if the observed sample mean $y_0$ matches with the model at parameter value $\theta_0$, and if the mapping $\theta \mapsto \mathbb{E}(Y_\theta)$ is one-to-one, then the law of large numbers implies that $y_0$ is an unlikely observation under any other parameter value $\theta \neq \theta_0$. In particular, $\theta_0$ will be a non-degenerate critical point, at least if we consider only the leading-order exponential factor as in (2.15). Conversely, if the gradient of $\theta \mapsto \mathbb{E}(Y_\theta)$ has rank $r < p$, there will be a $(p - r)$-dimensional surface around $\theta_0$ along which the mapping $\theta \mapsto \mathbb{E}(Y_\theta)$ is constant to first order. Hence, for all $\theta$ along this surface, $\hat{s}(\theta; y_0) \approx 0$ continues to be an approximate solution of the saddlepoint equation, the leading-order coefficient $K_0(\hat{s}; \theta) - \hat{s}y_0$ remains zero to first order, and the heuristic from Section 2.5.3 fails.

### 2.5.5 Observing multiple samples

As remarked in Section 2.2, the parameter $n$ should not be interpreted as a sample size in the traditional sense since the summands $Y^{(1)}, \ldots, Y^{(n)}$ of (2.9) are not observed. The usual large-sample limit refers to a model in which, instead of a vector $X$ of fixed dimension, we are given a vector $\vec{X}$ of dimension $km$ containing a large number $k$ of sub-blocks $X^{(1)}, \ldots, X^{(k)} \in \mathbb{R}^m$. In a large-sample limit, we model $X^{(1)}, \ldots, X^{(k)}$ as independent random variables with a common parametric distribution $X_\theta$, and we consider the limit $k \to \infty$ with $n$ fixed.

When we apply the saddlepoint approximation to the concatenated vector $\vec{X}$ of dimension $km$, the covariance matrix $K''_{\vec{X}}(\vec{s})$ will be block-diagonal. (In the language of Section 3, the tilting step preserves the independence of the $k$ sub-blocks.) It follows that the saddlepoint approximation for $\vec{X}$ factors as a product of $k$ $m$-dimensional saddlepoint approximations for $X^{(1)}, \ldots, X^{(k)}$. However, $n$ is fixed, so the individual saddlepoint approximations – each of which is a saddlepoint approximation applied to the distribution $X_\theta$ – need not be exact.

We now turn to the limit $k \to \infty$. In a setup similar to that of Theorem 4, write $\vec{x}_k \in \mathbb{R}^{km}$ for the random variable representing the observed data. Fix a parameter $\theta_0$ and suppose that $\vec{x}_k$ is the concatenation of $k$ vectors $x^{(1)}, \ldots, x^{(k)}$ drawn independently
with distribution $X_{\theta_0}$. In other words, suppose that the underlying model is well-specified relative to the data-generating process. Then, under typical conditions, we can expect to find that the true MLE is consistent, $\theta_{\text{MLE}}(\bar{x}) \to \theta_0$ in probability as $k \to \infty$.

However, the model corresponding to the saddlepoint likelihood $\hat{L}(\theta, \bar{x})$ is different, and in general will be mis-specified relative to the data-generating process. (That is, we assume that there is a parametric model whose likelihood has the form $\hat{L}(\theta, \bar{x}) = c(\bar{x})\tilde{L}(\theta; \bar{x})$.) Again under typical conditions, we can expect to find that the saddlepoint MLE converges in probability as $k \to \infty$ to some $\theta_1$, which will be the parameter that minimizes the relative entropy of the data-generating distribution $X_{\theta_0}$ relative to the distribution implied by $\hat{L}(\theta_1; \bar{x})$. However, there is no reason to expect $\theta_1$ to equal $\theta_0$.

In short, in the limit $k \to \infty$ we expect both true and saddlepoint MLEs to concentrate with increasing precision, but with $n$ fixed there is no reason to expect the saddlepoint MLE to concentrate around the correct limiting value.

### 2.5.6 Analogy to Fisher information and Godambe information

In the traditional large-sample limit, $k$ samples from the distribution $X_{\theta_0}$ are observed. In the basic result for convergence of the MLE, the resulting MLE is asymptotically normally distributed around the true parameter $\theta_0$, with a spatial scale $1/\sqrt{k}$. A principal assumption for this result is that the Fisher information matrix, which is positive semi-definite by construction, should be non-singular. In our setting, as discussed in Section 2.5.4, the analogue of this hypothesis is the requirement that the matrix in (2.45) should have full rank. However, these hypotheses are not the same: for instance, if changing $\theta$ causes the variance of $X_{\theta}$ to change but not the mean, this will be detectable in the Fisher information matrix but not in (2.45).

In general, it may not be reasonable to assume that our observations are drawn according to our model with an unknown parameter: that is, our model may be mis-specified. In the large-sample limit, the MLE is still normally distributed with a spatial scale $1/\sqrt{k}$, see for instance [18], with the requirement that the Godambe information matrix, rather than the Fisher information matrix, should be non-singular. In our setting, the analogue is the requirement (2.18) that the Hessian of (2.15) should be negative definite. The non-singularity of the Godambe information matrix is still, however, a different hypothesis than (2.18).

### 3 Tilting and the saddlepoint approximation

In Section 3.1 we break down the saddlepoint approximation into two steps: an exact step based on tilting, and an approximation step based on the normal distribution. Because the tilting step is exact, we can use the results of tilting to analyse both the true likelihood and the saddlepoint approximation.

Specifically, we factor the likelihood into an exact factor, which encodes the effect of tilting and is shared between the true and approximate likelihoods; and a correction term, a normal approximation of which leads to the saddlepoint likelihood. This factorization establishes the framework in which the proofs will take place, and also gives insight into results from the literature and possibly future directions of inquiry.

As a natural by-product of the factorization, we introduce in Section 3.2 a simpler but less accurate alternative to the saddlepoint approximation, which satisfies results similar to Theorems 1–5.
3.1 The saddlepoint approximation in two steps

If $X$ has density function $f$, the MGF $M(i\varphi)$ along the imaginary axis gives the Fourier transform of $f$. Consequently we can use the inverse Fourier transform to recover $f$:

$$f(x) = \int_{\mathbb{R}^{1 \times m}} M(i\varphi) e^{-ix\varphi} \frac{d\varphi}{(2\pi)^m} = \int_{\mathbb{R}^{1 \times m}} \exp \left( (K(i\varphi) - i\varphi x) \frac{d\varphi}{(2\pi)^m} \right). \quad (3.1)$$

As we will explain later, our assumptions imply that, for sufficiently large $n$, the integral in (3.1) converges absolutely and defines a continuous density function $f(x)$.

In practice, either of the factors $M(i\varphi)$ or $e^{-ix\varphi}$ may be highly oscillatory, and will not typically cancel with each other. To make the integral more manageable, we exponentially tilt the distribution of $X$. Define

$$f_{s_0}(x; \theta) = \frac{e^{s_0 x} f(x; \theta)}{M(s_0; \theta)} \quad (3.2)$$

for all $s_0 \in S_\theta$. Then $f_{s_0}$ is still a density function, corresponding to a tilted distribution $X(s_0)$ having the same support as $X$, and we compute

$$M_{X(s_0)}(s) = \frac{M(s_0 + s)}{M(s_0)}, \quad K_{X(s_0)}(s) = K(s_0 + s) - K(s_0). \quad (3.3)$$

Recalling (2.6), we note that $K'(s_0) = \mathbb{E}(X(s_0))$ and $K''(s_0) = \text{Cov}(X(s_0), X(s_0))$, so that $K''(s_0)$ is positive semi-definite for all $s_0 \in \text{int} S_\theta$. Since $X$ and $X(s)$ have the same support, we note from (2.7) that $K''(s_0)$ is positive definite for all $s_0 \in \text{int} S_\theta$. We will use this conclusion without further mention in the rest of the paper.

If we apply the inversion formula (3.1) to $X(s)$, we can solve to find

$$f(x) = M(s)e^{-sx}f_s(x)$$

$$= \exp \left( (K(s) - sx) \int_{\mathbb{R}^{1 \times m}} \exp \left( (K(s + i\varphi) - K(s) - i\varphi x) \frac{d\varphi}{(2\pi)^m} \right) \right). \quad (3.4)$$

Note that we can choose $s \in S_\theta$ arbitrarily. To make the integral more tractable, we wish to choose $s$ so that the linear term $-i\varphi x$ cancels with $K(s + i\varphi) - K(s)$ to leading order. That is, we choose $s = \hat{s}$, the solution of (SE), provided that $x \in \mathcal{X}_\theta$. Replacing $x$ by $K'(\hat{s})$, we have

$$f(x) = \exp \left( (K(\hat{s}) - \hat{s}K'(\hat{s})) \int_{\mathbb{R}^{1 \times m}} \exp \left( (K(\hat{s} + i\varphi) - K(\hat{s}) - i\varphi K'(\hat{s})) \frac{d\varphi}{(2\pi)^m} \right) \right). \quad (3.5)$$

Note at this point that explicit $x$ dependence has been virtually eliminated from (3.5); all $x$ dependence on the right-hand side is now carried implicitly by $\hat{s}$. We introduce new notation to exploit this feature. Along with this new notation, we again switch from considering the density $f$ to the likelihood $L$.

Define

$$L^*(\theta, s) = \exp \left( (K(s; \theta) - sK'(s; \theta)) \right),$$

$$P(\theta, s) = \int_{\mathbb{R}^{1 \times m}} \exp \left( (K(s + i\varphi) - K(s) - i\varphi K'(s)) \right) \frac{d\varphi}{(2\pi)^m}. \quad (3.6)$$

for all $s \in \text{int} S_\theta$. Setting $x = K'(s; \theta)$, (3.5) can be reformulated as

$$L(\theta; K'(s; \theta)) = L^*(\theta, s)P(\theta, s). \quad (3.7)$$
We can recognise log $L^*(\theta, s)$ as the negative of the relative entropy (or Kullback-Leibler divergence) for the distribution of $X_\theta^{(s)}$ relative to $X_\theta$. We can also give a probabilistic interpretation of $P(\theta, s)$: it is the density of the tilted distribution $X_\theta^{(s)}$ at its mean $K'(s; \theta)$.

We emphasise at this point that all the calculations so far are exact. The factor $L^*$ measures the probabilistic “cost” of shifting from the original distribution $X_\theta$ to the tilted distribution $X_\theta^{(s)}$, but no distributional information is lost in the tilting step.

The natural next step will be to make an approximation to $P(\theta, s)$. Define

$$
\hat{P}(\theta, s) = \frac{1}{\sqrt{\det(2\pi K''(s; \theta))}}.
$$

Then the saddlepoint approximation (SPA) becomes

$$
\hat{L}(\theta; K'(s; \theta)) = L^*(\theta, s)\hat{P}(\theta, s).
$$

We recognise $\hat{P}(\theta, s)$ as the density (at its mean) of a normal random variable with covariance matrix $K''(s; \theta)$. Comparing (3.7) and (3.9), we see that the saddlepoint approximation amounts to approximating $P(\theta, s)$, the density at its mean of the tilted distribution, by $\hat{P}(\theta, s)$, the density at its mean of the normal random variable with the same covariance matrix.

In the remainder of the paper, we will study the two-variable functions $L^*(\theta, s)$, $P(\theta, s)$ and $\hat{P}(\theta, s)$ and their gradients. Since the factor $L^*(\theta, s)$ appears in both (3.7) and (3.9), it will suffice to compare the gradients of $P$ and $\hat{P}$. Ultimately our interest will be in the case $s = \hat{s}(\theta; x)$, and we will therefore rewrite (3.7) and (3.9) as

$$
L(\theta; x) = L^*(\theta, \hat{s}(\theta; x))P(\theta, \hat{s}(\theta; x)),
$$

$$
\hat{L}(\theta; x) = L^*(\theta, \hat{s}(\theta; x))\hat{P}(\theta, \hat{s}(\theta; x)),
$$

for $x \in X_\theta$.

**Remark.** A key advantage to studying $L^*(\theta, s)$, $P(\theta, s)$ and $\hat{P}(\theta, s)$ is that, because $P$ and $\hat{P}$ both represent densities at the mean, they vary less dramatically as a function of their arguments than the full likelihoods $L(\theta; x)$ and $\hat{L}(\theta; x)$, even in the limit $n \to \infty$ from (SAR). As we shall see, both $P$ and $\hat{P}$ and their gradients behave asymptotically as powers of $n$. The only factor that decays exponentially in $n$ is $L^*$, and since it is a common factor of $L(\theta; x)$ and $\hat{L}(\theta; x)$ we can circumvent its effects.

The representation (3.10) is also useful for numerical calculation. Recent work by Lunde, Kleppe & Skaug [14] calculates densities and likelihoods to high relative precision, even in the tails, using saddlepoint methodology. Expressed in our notation, they evaluate $P(\theta, s)$ by applying a quadrature rule to the integral in (3.6). Because $P(\theta, s)$ is a density at the mean, the integral defining $P(\theta, s)$ is much more amenable to numerical integration than the inverse Fourier integral (3.1)

Likewise, the fact that $P$ and $\hat{P}$ both represent densities at the mean helps to explain why the saddlepoint approximation can be so accurate even in the tails. Given $x$ close to the boundary of $X_\theta$ (or tending to infinity), the corresponding saddlepoint $\hat{s}$ will be close to the boundary of $S_\hat{q}$ (or will tend to infinity). In such a limit, there is no reason in general to expect the ratio $\hat{P}/P$ to converge to 1; but often the density at the mean remains on the order of the inverse of the standard deviation, so that $\hat{P}/P$ may remain bounded. By contrast, normal approximations and other similar techniques rely on extrapolating a density far from the mean, and such an extrapolation can only be accurate if the true density happens to have the same tail behaviour far from the mean.
\( L^* \) and \( P \) in the integer-valued case  

When \( X \in \mathbb{Z}^{m \times 1} \), the analogue of (3.1) is

\[
\mathbb{P}(X = x) = \int_{[-\pi,\pi]^{m \times 1}} M(i\varphi)e^{-i\varphi x} \frac{d\varphi}{(2\pi)^m} \quad \text{for } x \in \mathbb{Z}^{m \times 1}. \quad (3.11)
\]

We can repeat the tilting argument above, leading us to define

\[
P_{\text{int}}(\theta, s) = \int_{[-\pi,\pi]^{m \times 1}} \exp \left( K(s + i\varphi) - K(s) - i\varphi K'(s) \right) \frac{d\varphi}{(2\pi)^m}. \quad (3.12)
\]

At integer values \( x \in \mathbb{Z}^{m \times 1} \), we take the likelihood function to be \( L(\theta; x) = \mathbb{P}(X_\theta = x) \), and we will have

\[
L(\theta; x) = L^*(\theta, \hat{s}(\theta; x))P_{\text{int}}(\theta, \hat{s}(\theta; x)). \quad (3.13)
\]

However, \( P_{\text{int}}(\theta, s) \) is defined whenever \((s, \theta) \in \text{int } S\). Thus we can use (3.13) as a definition of \( L(\theta; x) \) even when \( x \) is non-integer, although \( L(\theta; x) \) may not represent a probability in that case.

### 3.2 A lower-order saddlepoint approximation

Approximating \( P \) using first and second moments is a natural and reasonable step, but is not the only possible approach. As we have seen, the standard saddlepoint approximation selects a density from the family of normal distributions after matching first and second moments. An alternative is to use a different reference family of distributions: this is one approach to non-Gaussian saddlepoint approximations, originally developed by Wood, Booth & Butler [20] in a different context and with different tools.

An even simpler alternative, however, is to ignore \( P \) altogether. Define

\[
\hat{L}^*(\theta; x) = L^*(\theta, \hat{s}(\theta; x)) \quad (3.14)
\]

for \( x \in X_\theta \). We could describe \( \hat{L}^*(\theta; x) \) as the “zeroth-order” saddlepoint approximation to the likelihood. We saw the quantity \( \frac{1}{n} \log \hat{L}^*(\theta; x) \) and its derivatives in (2.15) and (2.17)–(2.18), and \( I_\theta(x) = -\log \hat{L}^*(\theta; x) \) is the large deviations rate function from Cramér’s theorem applied to \( X_\theta \). Equivalently, \( -\log \hat{L}^*(\theta; \cdot) \) is the Legendre transform of \( K(\cdot; \theta) \); see for instance [9, sections I.4 and V.1] or [12, section 1.2].

Form the corresponding maximum likelihood estimator

\[
\hat{\theta}^*_{\text{MLE}}(x) = \arg\max_\theta \hat{L}^*(\theta; x) \quad (3.15)
\]

when it exists, and likewise define \( \hat{\theta}^*_{\text{MLE}}|_{U,x} \) as in (2.21) with \( \hat{L} \) replaced by \( \hat{L}^* \). We remark that in the standard asymptotic regime (SAR) where \( x = ny \), the MLE \( \hat{\theta}^*_{\text{MLE}}(x) \) depends on \( y \) but not on \( n \); the same is true if we maximise over \( \theta \) restricted to a neighbourhood \( U \).

Applied to \( \hat{L}^* \), the conclusions of Theorems 1–5 are almost unchanged, except that error terms have powers of \( n \) changed by one:

**Proposition 14** (Zeroth-order saddlepoint approximation).

(a) Under the hypotheses of Theorem 1,

\[
\nabla_\theta \log \hat{L}^*(\theta; x) = \nabla_\theta \log L(\theta; x) + O(1) \quad \text{as } n \to \infty, \quad (3.16)
\]

with uniformity if \((y, \theta)\) is restricted to a compact subset of \( \text{int } Y \).
(b) Under the hypotheses of Theorems 2–3, there exist \(n_0 \in \mathbb{N}\) and neighbourhoods \(U \subset \mathbb{R}\) of \(\theta_0\) and \(V \subset \mathbb{R}^{m \times 1}\) of \(y_0\) such that, for all \(n \geq n_0\) and \(y \in V\), the function \(\theta \mapsto \hat{L}^*(\theta;x)\) has a unique local maximizer in \(U\) and, writing this local maximizer as \(\hat{\theta}_{\text{MLE in } U}(x)\),

\[
\left| \hat{\theta}_{\text{MLE in } U}(x) - \theta_{\text{MLE in } U}(x) \right| = O\left(1/n\right) \quad \text{as } n \to \infty.
\]

(3.17)

(c) Moreover, under \(\hat{\pi}^*_{U,x}\) with \(x = ny_0\),

\[
\sqrt{n} (\Theta - \theta_0) \xrightarrow{d} \mathcal{N}(0, -H^{-1}) \quad \text{as } n \to \infty,
\]

where \(H\) is the negative definite matrix from (2.18).

(d) Under the hypotheses of Theorem 4,

\[
\sqrt{n} \left( \hat{\theta}_{\text{MLE in } U}(\xi_n) - \theta_0 \right) \xrightarrow{d} Z \quad \text{as } n \to \infty,
\]

where \(Z\) is as in Theorem 4(a). Moreover the convergence occurs jointly with the convergence from Theorem 4(a), with the same limiting random variable \(Z\) in all cases.

(e) The above results also apply under the hypotheses of Theorem 5.

(f) Suppose \(X\) is the sufficient statistic for an exponential family indexed by the natural parameter \(\eta\). Let \(\hat{\eta}^*_{\text{MLE}}(x)\) be the parameter obtained by maximising \(\hat{L}^*\), provided the maximiser exists. Then \(\hat{\eta}^*_{\text{MLE}}(x)\) coincides with the true MLE.

It is notable that maximizing \(\hat{L}^*\) results in an approximation to the MLE whose error as \(n \to \infty\) is still smaller than the spatial scale \(1/\sqrt{n}\), even though \(\hat{L}^*\) is no longer an adequate approximation to the likelihood itself in the sense that \(\hat{L}^*/L \to \infty\) as \(n \to \infty\).

The proofs of (a)–(e) are given along with the corresponding proofs of Theorems 1–5. Part (f) holds by the same reasoning as Example 7: in the first factor in (2.31), we now remove the denominator, and the resulting factor still does not depend on \(\eta\).

4 Proofs of Theorems 1–2

The proof of Theorem 1 is based on two key results, Proposition 15 and Corollary 17, that refine the statement of Theorem 1 using the factorisation from Section 3.1. Theorem 2 follows using a scaling analysis and the Implicit Function Theorem. We begin with some derivative formulas; see Appendix B for their derivation.

4.1 Summary of saddlepoint derivatives

Under the scaling of (SAR), the quantities \(\log \hat{L}^*(\theta,s), \log \hat{L}^*(\theta,\hat{s}(\theta;x))\) and their gradients are proportional to \(n\). Define

\[
L_0^*(\theta,s) = \exp \left( K_0(s;\theta) - sK_{0}'(s;\theta) \right),
\]

\[
\hat{L}_0(\theta;y) = L_0(\theta,\hat{s}_0(\theta;y)) = \exp \left( K_0(\hat{s}_0(\theta;y);\theta) - \hat{s}_0(\theta;y)y \right),
\]

(4.1)
so that
\[ \log L^*(\theta, s) = n \log L_0^*(\theta, s), \quad \nabla_\theta \log L_0^*(\theta; x) = n \nabla_\theta \log L_0^*(\theta; y) \tag{4.2} \]
and so on, where
\[ \nabla_\theta \log L_0^*(\theta, s) = \nabla_\theta K_0(s; \theta) - s \nabla_s \nabla_\theta K_0(s; \theta), \]
\[ \nabla_s \log L_0^*(\theta, s) = -K'_{0s}(s; \theta) s^T, \]
\[ \nabla_\theta \log \hat{L}_0^*(\theta; y) = \nabla_\theta K_0(\hat{s}_0(\theta; y); \theta), \]
\[ \nabla_\theta^T \nabla_\theta \log \hat{L}_0^*(\theta; y) = \nabla_\theta^T \nabla_\theta K_0(\hat{s}) - (\nabla_s \nabla_\theta K_0(\hat{s}))^T K_0''(\hat{s})^{-1} \nabla_s \nabla_\theta K_0(\hat{s}) \tag{4.3} \]

By contrast, \( \hat{s}, \nabla_\theta \hat{s}^T \) and \( \frac{\partial}{\partial t} \log \hat{P} \) do not depend on \( n \):
\[ \hat{s}(\theta; x) = \hat{s}_0(\theta; y), \]
\[ \nabla_\theta \hat{s}^T(\theta; x) = \nabla_\theta \hat{s}_0^T(\theta; y) = -K'_{0s}(\hat{s}(\theta; x); \theta)^{-1} \nabla_s \nabla_\theta K_0(\hat{s}(\theta; x); \theta), \]
\[ \frac{\partial}{\partial t} \log \hat{P}(\theta, s) = -\frac{1}{2} \text{tr} \left( K''_{0s}(s; \theta)^{-1} \frac{\partial K''_{0s}(s; \theta)}{\partial t} \right). \tag{4.4} \]

For the remainder of the proofs, we will emphasise that \( P(\theta, s), P_{\text{int}}(\theta, s), L(\theta; x), \hat{L}(\theta; x), \theta_{\text{MLE}}(x), \theta_{\text{MLE}}(x) \) depend on \( n \) by writing them as \( P_n(\theta, s), P_{\text{int}, n}(\theta, s), L_n(\theta; x), \hat{L}_n(\theta; x), \theta_{\text{MLE}}(x, n), \theta_{\text{MLE}}(x, n) \). The \( n \)-dependences of \( M(s; \theta), K(s; \theta), \log L^* \) and \( \log \hat{L}^* \) are simple in form and we will handle them by directly substituting the formulas in (SAR) and (4.2). We remark that the expression in (2.15) reduces to \( \log \hat{L}_0^*(\theta; y_0) \), and (2.17)–(2.18) amount to the assertion that \( \theta_0 \) is a non-degenerate critical point for \( \theta \mapsto \log \hat{L}_0^*(\theta; y_0) \).

Note that \( \hat{P}_n(\theta, s) \) also depends on \( n \) in a simple way,
\[ \hat{P}_n(\theta, s) = \frac{1}{\sqrt{\det(2\pi nK_0''(s; \theta))}} = \frac{n^{-m/2}}{\sqrt{\det(2\pi K_0''(s; \theta))}}. \tag{4.5} \]

but by (4.4) the gradients \( \nabla_s \log \hat{P}(\theta, s), \nabla_\theta \log \hat{P}(\theta, s) \) do not depend on \( n \) and we will omit the subscript in those cases.

### 4.2 Proof of Theorem 1

Unlike \( L^* \) and \( \hat{P}_n \), the quantity \( P_n \) has no closed form and is instead given as an integral as in (3.6). In the standard asymptotic regime given by (SAR), we can substitute \( K = nK_0 \) to obtain
\[ P_n(\theta, s) = \int_{\mathbb{R}^{1 \times m}} \exp \left( n[K_0(s + i\varphi) - K_0(s) - i\varphi K_0'(s)] \right) \frac{d\varphi}{(2\pi)^m}. \tag{4.6} \]

Note that the integrand in (4.6) has the form \( h(\varphi)e^{ng(\varphi)} \) with \( g(0) = 0 \) and \( g'(0) = 0 \). This is the standard setup for applying the multivariate Laplace method, see [19, 4]. Thus the limiting framework of (SAR), in which \( X \) is the sum of \( n \) i.i.d. terms, leads us to expect that \( P_n(\theta, s) \), after suitable rescaling by a power of \( n \), will have an asymptotic series expansion in powers of \( 1/n \).

Let the scalar \( t \) denote one of the coordinates \( \theta_i \) or \( s_j \). As we will show later, for large enough \( n \) we may differentiate under the integral sign:
\[ \frac{\partial P_n}{\partial t}(\theta, s) = \int_{\mathbb{R}^{1 \times m}} \exp \left( n[K_0(s + i\varphi) - K_0(s) - i\varphi K_0'(s)] \right) \cdot \left[ n \left[ \frac{\partial K_0}{\partial t}(s + i\varphi) - \frac{\partial K_0}{\partial t}(s) - i\varphi \frac{\partial K_0'}{\partial t}(s) \right] \right] \frac{d\varphi}{(2\pi)^m}. \tag{4.7} \]
A key observation motivating Theorem 1 is that $\frac{\partial P_n}{\partial t}(\theta, s)$ scales according to the same $n$-dependent factor as $P_n(\theta, s)$. Indeed, the values of both integrals arise primarily from the region where $\varphi$ is of order $1/\sqrt{n}$, and the extra factor in (4.7) is of order 1 in that region. We could summarise by saying that taking gradients of $P_n(\theta, s)$ with respect to $\theta$ or $s$ does not substantially change the nature of the $n$-dependence.

When we turn to MLEs, we will need to control the dependence of $P_n(\theta, s)$ (and its gradients) on $\theta$, $s$ and $n$ simultaneously. Specifically, the proof of Theorem 2 is based on the Implicit Function Theorem, which requires continuous differentiability. We will therefore prove the following result, which is more precise than is necessary for Theorem 1.

**Proposition 15.** Under the hypotheses of Theorem 1, with $t$ being one of the entries $\theta$, or $s_j$, there are continuously differentiable functions $q_1(\theta, s, \varepsilon)$, $q_2(\theta, s, \varepsilon)$, defined on an open set $Q$ containing $\{(\theta, s, 0) : (s, \theta) \in \text{int} S\}$, such that $q_1(\theta, s, 0) = q_2(\theta, s, 0) = 0$ and

$$\frac{\partial P_n}{\partial t}(\theta, s) = \frac{\partial P_n}{\partial t}(\theta, s) \left(1 + q_1(\theta, s, 1/n)\right)$$

whenever $n$ is large enough that $(\theta, s, 1/n) \in Q$.

An almost identical statement holds in the integer-valued case:

**Proposition 16.** Under the hypotheses of Theorem 5, the conclusions of Proposition 15 hold with $P(\theta, s)$ replaced by $P_{\text{int}}(\theta, s)$.

The proofs of Propositions 15–16 use many of the elements of standard proofs of Laplace's method. Additional care is needed to ensure that $q_1, q_2$ are continuously differentiable, and we defer the details to Appendix C.

Everything we will use from Propositions 15–16 can be encapsulated in the following corollary, or its analogue for $P_{\text{int}}(\theta, s)$.

**Corollary 17.** Under the hypotheses of Theorem 1, there is a continuously differentiable function $q_3(\theta, y, \varepsilon)$, with values in $\mathbb{R}^{1 \times p}$, defined on an open set $Q'$ containing $\{(\theta, s, 0) : (s, \theta) \in \text{int} S\}$, such that $q_3(\theta, y, 0) = 0$ and

$$\nabla_\theta \left(\log P_n(\theta, \hat{s}_0(\theta, y))\right) = \nabla_\theta \left(\log \hat{P}(\theta, \hat{s}_0(\theta, y))\right) + q_3(\theta, y, 1/n)$$

whenever $(\theta, s, 1/n) \in Q'$.

The proof is again deferred to Appendix C. Theorem 1 now follows immediately.

**Proof of Theorem 1.** Use (3.10) and cancel the factor $L^*$ to obtain

$$\nabla_\theta \log L(\theta; x) - \nabla_\theta \log \hat{L}(\theta; x) = \nabla_\theta \left(\log P_n(\theta, \hat{s}_0(\theta; y))\right) - \nabla_\theta \left(\log \hat{P}(\theta, \hat{s}_0(\theta; y))\right)$$

$$= q_3(\theta, y, 1/n).$$

By Corollary 17, $q_3$ is continuously differentiable and $q_3(\theta, y, 0) = 0$. An application of the Mean Value Theorem completes the proof.

The first assertion of Proposition 14 also follows easily:

**Proof of Proposition 14(a).** Since Theorem 1 already gives a bound on $\nabla_\theta \log \hat{L} - \nabla_\theta \log L$, it suffices to show that $\nabla_\theta \log \hat{L} - \nabla_\theta \log \hat{L} = O(1)$. From (3.10) and (4.4), $\nabla_\theta \log (\hat{L}(\theta; x)/\hat{L}^*(\theta; x)) = \nabla_\theta \log \hat{P}(\theta, \hat{s}_0(\theta; y))$ is constant with respect to $n$, so it is $O(1)$ in the limit $n \to \infty$. Since it also depends continuously on $\theta$ and $y$, uniformity follows.
4.3 Proof of Theorem 2

To study the MLE $\theta_{\text{MLE in } U}(x, n)$, we will show that the function $\theta \mapsto \log L_n(\theta; x)$ has a unique maximum when $\theta$ is restricted to lie in a suitably chosen neighbourhood $U$. In fact it will be more convenient to consider the rescaled function

$$R_{x,n}(\theta) = \frac{1}{n} \log L_n(\theta; x) = L_0'(\theta, \hat{s}_0(\theta; y)) + \frac{1}{n} \log P_n(\theta, \hat{s}_0(\theta; y)), \quad (4.11)$$

where we have substituted (3.10) and (4.2). Use (4.4) and Corollary 17 to compute

$$R'_{x,n}(\theta) = \nabla_\theta K_0(\hat{s}_0(\theta; y); \theta) + \frac{1}{n} g_3(\theta, y, 1/n) + \frac{1}{n} \nabla_\theta \log \hat{P}(\theta, \hat{s}_0(\theta; y))$$

$$- \frac{1}{n} \nabla_s^T \log \hat{P}(\theta, \hat{s}_0(\theta; y)) K_0'(\hat{s}_0(\theta; y); \theta)^{-1} \nabla_s \nabla_\theta K_0(\hat{s}_0(\theta; y); \theta). \quad (4.12)$$

Recalling the change of variables $\varepsilon = 1/n$, we will define a function $F(s^T, \theta, y, \varepsilon)$ such that a solution of $F = 0$ corresponds to a critical point of $R_{x,n}$.

**Proof of Theorem 2.** Define the functions

$$F(s^T, \theta, y, \varepsilon) = \begin{pmatrix} F_1(s^T, \theta, y) \\ F_2(s^T, \theta, y, \varepsilon) \end{pmatrix}, \quad F_1(s^T, \theta, y) = K_0'(s; \theta) - y,$$  

$$F_2(s^T, \theta, y, \varepsilon) = \nabla_\theta^T K_0(s; \theta) + \varepsilon g_3(\theta, y, \varepsilon)^T$$

$$+ \varepsilon \left( \nabla_\theta^T \log \hat{P}(\theta, s) - (\nabla_s \nabla_\theta K_0(s; \theta))^T K_0''(s; \theta)^{-1} \nabla_s \log \hat{P}(\theta, s) \right). \quad (4.13)$$

We think of $F_1, F_2, F$ as column-vector-valued functions of column-vector arguments, with $(s^T, \theta, y, \varepsilon)$ and $F(s^T, \theta, y, \varepsilon)$ interpreted as column vectors expressed in block form, of sizes $(2m + p + 1) \times 1$ and $(m + p) \times 1$ respectively. We will show that we can solve $F = 0$ to define $\theta$ and $s$ implicitly as functions of $y$ and $\varepsilon$; to indicate this, we will merge the column vectors $s^T$ and $\theta$ and write $\begin{pmatrix} s^T \\ \theta \end{pmatrix} = G(y, \varepsilon) \in \mathbb{R}^{(m+p)\times 1}$ such that $F(G(y, \varepsilon); y, \varepsilon) = 0$.

By Corollary 17, the function $F$ is continuously differentiable with respect to all its parameters. Our assumptions imply that $F(s^T_0, \theta_0; y_0, 0) = 0$ and $\nabla_{s^T, \theta} F(s^T_0, \theta_0; y_0, 0)$ is non-singular; see Appendix E. We can therefore apply the Implicit Function Theorem to find neighbourhoods $U, V, W$ of $\theta_0, y_0, s_0$, a neighbourhood $[-1/n_0, 1/n_0]$ of 0, and a continuously differentiable function $G(y, \varepsilon)$ defined on $V \times [-1/n_0, 1/n_0]$ such that, for all $y \in V$, $\varepsilon \in [-1/n_0, 1/n_0]$, the point $\begin{pmatrix} s^T \\ \theta \end{pmatrix} = G(y, \varepsilon)$ is the unique solution in $U \times W$ of $F(s^T, \theta, y, \varepsilon) = 0$.

Finally, as outlined above, when $\varepsilon = 1/n$, the solution of $F = 0$ corresponds to the MLE:

**Lemma 18.** Possibly after shrinking $U, V$ and increasing $n_0$, we have

$$G(y, 1/n) = \begin{pmatrix} \hat{s}_0^T(\theta_{\text{MLE in } U}(x, n); y) \\ \theta_{\text{MLE in } U}(x, n) \end{pmatrix} \quad (4.14)$$

for all $y \in V$ and $n \geq n_0$, including the assertion that the maximum of $L_n(\theta; x)$, restricted to $\theta \in U$, is attained uniquely.

We defer the proof to Appendix E.
We now turn to the saddlepoint MLE, which amounts to omitting the term \( \varepsilon q_3 \):
\[
\tilde{F}_2(s^T, \theta; y, \varepsilon) = \nabla^T_{\theta} K_0(s; \theta) + \varepsilon \nabla^T_{\theta} \log \hat{P}(\theta, s) - \varepsilon (\nabla_{s} \nabla_{\theta} K_0(s; \theta))^T K_0''(s; \theta)^{-1} \nabla_{s} \log \hat{P}(\theta, s),
\]
\[
\tilde{F}(s^T, \theta; y, \varepsilon) = \left( \frac{F_1(s^T, \theta; y)}{F_2(s^T, \theta; y, \varepsilon)} \right).
\] (4.15)

Then \( \tilde{F} \) and its gradients agree with \( F \) and its gradients at \((s_0^T, \theta_0; y_0, 0)\), so that (after shrinking \( U, V, W \) and increasing \( n_0 \) if necessary) the Implicit Function Theorem again produces a function \( \hat{G}(y, \varepsilon) \) giving the unique solution \( \left( s^T_0 \right)_\theta \) in \( U \times W \) of \( \hat{F}(s^T, \theta; y, \varepsilon) = 0 \). Moreover the analogue of Lemma 18 applies, with the same proof, so that
\[
\hat{G}(y, 1/n) = \left( \bar{\theta}^T_{\text{MLEinU}}(x, n) ; y \right).
\] (4.16)

For later convenience write \( \hat{G} \) in block form as \( \hat{G} = \left( \hat{G}_s^T \right. \left. \hat{G}_\theta \right) \).

To compare \( G(y, \varepsilon) \) with \( \hat{G}(y, \varepsilon) \), note that \( F_2 \) and \( \tilde{F}_2 \) are close:
\[
F_2(s^T, \theta; y, \varepsilon) = \tilde{F}_2(s^T, \theta; y, \varepsilon) + \varepsilon q_3(\theta, y, \varepsilon).
\] (4.17)

In particular, \( F(\hat{G}(y, \varepsilon); y, \varepsilon) \) is almost zero:
\[
F(\hat{G}(y, \varepsilon); y, \varepsilon) = \left( \begin{array}{c} F_1(\hat{G}(y, \varepsilon); y, \varepsilon) \\ \tilde{F}_2(\hat{G}(y, \varepsilon); y, \varepsilon) \end{array} \right) + \left( \begin{array}{c} 0 \\ \varepsilon q_3(\hat{\theta}_{\text{MLEinU}}(x, n) ; y) \end{array} \right).
\] (4.18)

The first term in the right-hand side vanishes by definition. In the second term, note that \( q_3(\hat{\theta}_{\text{MLEinU}}(x, n) ; y) \) is a continuously differentiable function of \((y, \varepsilon)\) that vanishes whenever \( \varepsilon = 0 \) (since \( q_3 \) has the same property by Corollary 17). We can therefore conclude that
\[
F(\hat{G}(y, \varepsilon); y, \varepsilon) = \varepsilon^2 q_4(y, \varepsilon)
\] (4.19)

where \( |q_4(y, \varepsilon)| \leq C \) for \((y, \varepsilon)\) in a suitable neighbourhood of \((y_0, 0)\).

To make use of (4.19), we define an augmented version of \( F \) that is locally invertible. Let
\[
\bar{F}(s^T, \theta; y, \varepsilon) = \left( \begin{array}{c} F(s^T, \theta; y, \varepsilon) \\ y \\ \varepsilon \end{array} \right), \quad \text{so that} \quad \nabla_{s^T, \theta, y, \varepsilon} \bar{F} = \left( \begin{array}{ccc} \nabla_{s^T, \theta} F & \nabla_y F & \nabla_{\varepsilon} F \\ 0 & I_{m \times m} & 0 \\ 0 & 0 & 1 \end{array} \right)
\] (4.20)
in block form. Thus \( \nabla_{s^T, \theta, y, \varepsilon} \bar{F}(s_0^T, \theta_0; y_0, 0) \) is an invertible \((2m + p + 1) \times (2m + p + 1)\) matrix, and by the Inverse Function Theorem [16, Theorem 9.24], after shrinking the domain of \( \bar{F} \) if necessary, \( \bar{F} \) has a continuously differentiable inverse function \( \hat{G}(u; y, \varepsilon) \).

As above, we may shrink the domain further to make the partial derivatives of \( \hat{G} \) uniformly bounded.

The inverse function \( \hat{G} \) is related to the implicit function \( G \) by \( \hat{G}(0; y, \varepsilon) = \left( \begin{array}{c} G(y, \varepsilon) \\ y \\ \varepsilon \end{array} \right) \).

From (4.19) and the definition of \( \bar{F} \) we have
\[
\bar{F}(\hat{G}(y, \varepsilon); y, \varepsilon) = \left( \begin{array}{c} \varepsilon^2 q_4(y, \varepsilon) \\ y \\ \varepsilon \end{array} \right) \quad \text{and so} \quad \hat{G}(\varepsilon^2 q_4(y, \varepsilon); y, \varepsilon) = \left( \begin{array}{c} G(y, \varepsilon) \\ y \\ \varepsilon \end{array} \right).
\] (4.21)
Thus, setting $\varepsilon = 1/n$ for $n$ sufficiently large,
\[
\left| \hat{\theta}_{\text{MLE}}(x, n) - \theta_{\text{MLE}}(x, n) \right| \leq \left| \hat{G}(y, 1/n) - G(y, 1/n) \right|
= \left| \hat{G}(n^{-2}q_4(y, 1/n); y, 1/n) - \hat{G}(0; y, 1/n) \right|.
\] (4.22)

The boundedness of $q_4$ and of the partial derivatives of $\hat{G}$ imply that this upper bound is $O(1/n^2)$, uniformly over $y$ in a suitable neighbourhood of $y_0$.

The corresponding assertion from Proposition 14 has a similar proof:

**Proof of Proposition 14(b).** Note that $\theta = \hat{\theta}^{*}_{\text{MLE}}(x, n)$ and $s = \hat{s}(\theta; x)$ are solutions of $F(s^T, \theta; y, 0) = 0$. (The proof is the same as for Lemma 18, with the relation $\nabla^2_{\theta} \hat{L}^*(\theta; x) = F_2(s^2_0(\theta; y), \theta; y, 0)$ in place of (E.4); see Appendix E.) Then
\[
\left| \hat{\theta}^{*}_{\text{MLE}}(x, n) - \theta_{\text{MLE}}(x, n) \right| \leq |G(y, 0) - G(y, 1/n)|
\] (4.23)
and the conclusion follows from the fact that $G$ is continuously differentiable.

## 5 Conclusion

A long-established result tells us that the saddlepoint approximation gives a relative error of order $1/n$. That is, applied to a random variable given as a sum of $n$ i.i.d. terms, the saddlepoint approximation estimates the values of the density (or likelihood) up to a factor of the form $1 + O(1/n)$: see (2.11) or Proposition 15. Very commonly, however, we are not interested in the likelihood for its own sake but rather as a step towards computing the MLE. This paper gives the analogous basic result, Theorem 2, for the approximation error between the true MLE and saddlepoint MLE: it is of order $1/n^2$.

It is worth mentioning that this MLE error estimate is sharper than what we obtain from the basic likelihood error estimate. Knowing that $\log \hat{L}(\theta; x)$ has a maximum at $\theta = \hat{\theta}_{\text{MLE}}(x)$ and knowing that the true log-likelihood satisfies $|\log \hat{L}(\theta; x) - \log \hat{L}(\theta; x)| = O(1/n)$, we can only conclude that $|\theta_{\text{MLE}}(x) - \hat{\theta}_{\text{MLE}}(x)| = O(1/n)$ (since this is the size of the region in which $\log \hat{L}$ is within $O(1/n)$ of its maximum). Although an MLE error bound of size $O(1/n)$ is small compared to the scale of the inferential uncertainty in estimating $\theta$, see Theorems 3–4 and the remarks at the end of Section 2.3, it is still a significant overestimate compared to the true MLE error $O(1/n^2)$. The results in this paper help to explain why saddlepoint MLEs in practice often turn out to be so much more accurate than expected.

A key point in the analysis is to ask how well the saddlepoint approximation captures the shape of the log-likelihood as a function of the parameter $\theta$. Specifically, it is error bounds on the gradient of the log-likelihood, as in Theorem 1 and Corollary 17, that control the size of the MLE approximation error. This is the logic behind the finding of Example 7 that saddlepoint MLEs are exact for exponential families: errors in the saddlepoint approximation to the log-likelihood are irrelevant if the size of the errors do not depend on the parameter.

Seen in this light, it is less surprising that a lower-order saddlepoint approximation, $\hat{L}^*(\theta; x)$ from Section 3.2, can give a good approximation to the MLE (see Proposition 14) despite being a poor approximation to the likelihood with $\hat{L}^*(\theta; x)/L(\theta; x) \to \infty$ as $n \to \infty$. We remark that since $\hat{L}^*(\theta; x)$ is even less computationally demanding than
the usual saddlepoint approximation, it may be a useful tool for high-dimensional and computationally intensive applications, or for initialising the search for a true or saddle-point MLE.

In the other direction, refinements of the saddlepoint approximation that improve likelihood accuracy may be less effective than anticipated when applied to MLEs. For instance, normalising the saddlepoint approximation $\hat{f}(x; \theta)$ to make it a density (as a function of $x$) often brings the saddlepoint density values closer to the true density (see for instance [5]). However, this operation is slow and is often not pursued; cf. [7]. Using the viewpoint developed in this paper, we can reframe the issue by asking: does normalising bring the saddlepoint log-gradient closer to the true log-gradient? The general answer is far from clear. Indeed, for an exponential family such as the Poisson family, for which the saddlepoint MLE is already exact as in Example 6, normalising will actually make the MLE worse.

This paper has considered likelihoods and MLEs in a particularly tractable limiting framework, the standard asymptotic regime (SAR) in which the observation is a sum of $n$ i.i.d. terms. In particular, we have seen that the basic likelihood accuracy estimate does not directly lead to the correct MLE error estimate, which is markedly better. It would be of interest to extend these results in several directions, including non-Gaussian saddlepoint approximations, as in [20]; non-i.i.d. sums; integer-valued random variables; exact upper bounds; and applications based on approximating tail probabilities rather than likelihoods.

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References


A  Invariance properties of the saddlepoint approximation

If \( b \in \mathbb{R}^{m \times 1} \) and \( Y = X + b \), the corresponding saddlepoint approximations are related by

\[
\hat{L}_Y(\theta; y) = \hat{L}_X(\theta; y - b), \tag{A.1}
\]

with the same saddlepoint \( \hat{s} \) in both approximations.

If \( A \in \mathbb{R}^{k \times m} \) and \( Z = AX \), then

\[
K_Z(s) = K_X(sA), \tag{A.2}
\]

and it follows that

\[
K''_Z(s) = AK''_X(s)A^T. \tag{A.3}
\]

In particular, if \( A \) is \( m \times m \) and invertible, then \( \det(K''_Z(s)) = \det(A)^2 \det(K''_X(s)) \) and

\[
\hat{L}_Z(\theta; z) = \frac{\hat{L}_X(\theta; A^{-1}z)}{|\det(\theta)|}, \tag{A.4}
\]

with the saddlepoints related by \( \hat{s}_Z = \hat{s}_X A^{-1} \).

Equations (A.1) and (A.4) show that, under invertible affine transformations of the random variables, the saddlepoint approximation transforms in the same way that densities do. In particular, such transformations will not affect the MLE or saddlepoint MLE, and in the standard asymptotic regime we may equivalently consider \( \hat{Y} = \frac{1}{n} \hat{X} \), the sample mean of the \( n \) unobserved values \( Y^{(1)}, \ldots, Y^{(n)} \), in place of \( X \). We have chosen to consider \( X \) because the saddlepoint for \( \hat{Y} \) scales with \( n \) for a fixed value of \( y \), whereas the saddlepoint for \( X \) does not.

B  Derivatives of saddlepoint quantities

We will need to differentiate the quantities \( \log L^* \), \( \hat{s} \), \( \log L^*(\theta, \hat{s}) \) and \( \hat{P} \). The first of these is simple since \( L^* \) is exact and explicitly computable:

\[
\nabla_\theta \log L^*(\theta, s) = \nabla_\theta K(s; \theta) - s \nabla_s \nabla_\theta K(s; \theta),
\]
\[
\nabla_s \log L^*(\theta, s) = K'(s; \theta) - K''(s; \theta) - K''(s; \theta) s^T = -K''(s; \theta) s^T. \tag{B.1}
\]

For \( \hat{s}(\theta; x) \), suppose \((s_0, \theta_0) \in \text{int} \mathcal{S} \) with \( K'(s_0; \theta_0) = x_0 \). The function \((s, \theta, x) \mapsto K'(s; \theta) - x \) is continuously differentiable and its gradient with respect to \( s^T \), i.e., \( K''(s; \theta) \), is positive definite and hence non-singular. Hence the Implicit Function Theorem (see for instance [16, Theorem 9.28]) implies that \( \hat{s}(\theta; x) \) is uniquely defined and continuously differentiable for \( \theta, x \) in a neighbourhood of \( \theta_0, x_0 \).

We next state two versions of the chain rule, which are slightly different for row vectors and column vectors. If \( f_{row}(s) : \mathbb{R}^{1 \times m} \to \mathbb{R}^{1 \times k} \) and \( g_{row}(v) : \mathbb{R}^{1 \times j} \to \mathbb{R}^{1 \times m} \) are differentiable then \( h_{row}(v) = f_{row}(g_{row}(v)) \) has

\[
\nabla_v h_{row}(v) = \nabla_v g_{row}(v) \nabla_s f_{row}(g_{row}(v)). \tag{B.2}
\]

Similarly, if \( f_{col}(t) : \mathbb{R}^{p \times 1} \to \mathbb{R}^{k \times 1} \) and \( g_{col}(w) : \mathbb{R}^{j \times 1} \to \mathbb{R}^{p \times 1} \) are differentiable then \( h_{col}(w) = f_{col}(g_{col}(w)) \) has

\[
\nabla_w h_{col}(w) = \nabla_t f_{col}(g_{col}(w)) \nabla_w g_{col}(w). \tag{B.3}
\]
We now find the gradients of $\hat{s}(\theta; x)$. Note that $\hat{s}(\theta; x)$ is a row-vector-valued function of column vector arguments. To match, we will consider the transpose $\hat{s}^T(\theta; x)$ instead, and to differentiate (SE) we will think of $K'(s; \theta) = \nabla_s K(s; \theta)$ as a column-vector-valued function of two column vector arguments, $\theta$ and $s^T$. Applying (B.3),

$$0 = \nabla_{\theta} x = \nabla_{\theta} \left( \nabla_s K(\hat{s}(\theta; x); \theta) \right)$$

$$= \nabla_s \nabla_{\theta} K(\hat{s}(\theta; x); \theta) + \nabla_s \nabla_{\theta}^T K(\hat{s}(\theta; x); \theta) \nabla_{\theta} \hat{s}^T(\theta; x). \quad \text{(B.4)}$$

Note our convention for gradients and composite functions: in (B.4), an expression such as $\nabla_s \nabla_{\theta} K(\hat{s}(\theta; x); \theta)$ means the $m \times p$ matrix of mixed partial derivatives $\frac{\partial^2 K}{\partial s_i \partial \theta_j}$ evaluated with $s$ replaced by $\hat{s}(\theta; x)$, whereas $\nabla_{\theta} \left( \nabla_s K(\hat{s}(\theta; x); \theta) \right)$ means the gradient of the composite function $\theta \mapsto \nabla_s K(\hat{s}(\theta; x); \theta)$. In (B.4), $\nabla_s \nabla_{\theta}^T K = \nabla_s \nabla_{\theta}^T K = K''$ is non-singular, so we can solve to find

$$\nabla_{\theta} \hat{s}^T(\theta; x) = -K''(\hat{s}(\theta; x); \theta)^{-1} \nabla_s \nabla_{\theta} K(\hat{s}(\theta; x); \theta) \quad \text{(B.5)}$$

Similarly, with $I_{m \times m}$ representing the $m \times m$ identity matrix,

$$I_{m \times m} = \nabla_{x} x = \nabla_{x} \left( \nabla_s K(\hat{s}(\theta; x); \theta) \right) = \nabla_s \nabla_{\theta}^T K(\hat{s}(\theta; x); \theta) \nabla_{x} \hat{s}^T(\theta; x) \quad \text{(B.6)}$$

so that

$$\nabla_{x} \hat{s}^T(\theta; x) = K''(\hat{s}(\theta; x); \theta)^{-1}. \quad \text{(B.7)}$$

Turning to log $\hat{L}^* (\theta; x) = \log L^* (\theta; x) - \hat{s}^T K'(\hat{s})$, recall that $K'(\hat{s}(\theta; x); \theta) = x$ by definition. Noting that $\hat{s} x = x^T \hat{s}^T$, we find that

$$\nabla_{\theta} \log \hat{L}^* (\theta; x) = \nabla_{\theta} \left( K(\hat{s}(\theta; x); \theta) - x^T \hat{s}^T \right)$$

$$= \nabla_{\theta} K(\hat{s}) + \nabla_{\theta}^T K(\hat{s}(\theta; x)) \nabla_{\theta} \hat{s}^T(\theta; x) - x^T \nabla_{\theta} \hat{s}^T(\theta; x)$$

$$= \nabla_{\theta} K(\hat{s}(\theta; x); \theta) \quad \text{(B.8)}$$

since $\nabla_{s^T} K(\hat{s}) = (\nabla_s K(\hat{s}))^T = x^T$. (Alternatively, use the relations (B.1).) Transposing then differentiating again,

$$\nabla_{\theta}^T \nabla_{\theta} \log \hat{L}^* (\theta; x) = \nabla_{\theta} \left( \nabla_{\theta} K(\hat{s}(\theta; x); \theta) \right)^T$$

$$= \nabla_{\theta}^T \nabla_{\theta} K(\hat{s}(\theta; x)) + \nabla_{\theta}^T \nabla_{\theta}^T K(\hat{s}(\theta; x); \theta) \nabla_{\theta} \hat{s}^T(\theta; x)$$

$$= \nabla_{\theta}^T \nabla_{\theta} K(\hat{s}) - (\nabla_s \nabla_{\theta} K(\hat{s}))^T K''(\hat{s})^{-1} \nabla_s \nabla_{\theta} K(\hat{s}). \quad \text{(B.9)}$$

Equations (B.8)–(B.9) verify the assertion before Theorem 2 that the quantities in (2.17)–(2.18) are the gradient and Hessian of the function in (2.15).

For log $\hat{P}$, we first show how to differentiate a determinant. Suppose that $A(t): \mathbb{R} \rightarrow \mathbb{R}^{m \times m}$ is a differentiable matrix-valued function of a scalar parameter $t$. Then

$$\frac{d}{dt} \log \det A(t) = \text{tr}(A(t)^{-1} A'(t)). \quad \text{(B.10)}$$

This formula appears as [17, Appendix M.7.f, equation (49)]. They derive the formula under the assumption that $A$ is symmetric, but the formula is true in all cases, and we include a proof for completeness. Supposing without loss of generality that we wish to differentiate at $t = 0$, write

$$A(t) = A_0 + t B(t) \quad \text{(B.11)}$$
with \( B(t) \) a continuous matrix-valued function, so that \( B(0) = A'(0) \). We are interested in the derivative of \( \log \det A(t) \) so we will suppose for convenience that \( \det A_0 \neq 0 \). Then

\[
\det A(t) = \det A_0 \det \left( I + tA_0^{-1}B(t) \right) = \det A_0 \left( 1 + t \tr(A_0^{-1}B(t)) + O(t^2) \right). \tag{B.12}
\]

To see this, recall the expansion

\[
\det \left( I + tA_0^{-1}B(t) \right) = \sum_\pi \sign(\pi) \prod_{i=1}^m (I + tA_0^{-1}B(t))_{i\pi(i)} \tag{B.13}
\]

where the sum is over permutations \( \pi \) of \( \{1, 2, \ldots, m\} \). If \( \pi \) is different from the identity permutation, then at least two of the pairs \((i, \pi(i))\) refer to off-diagonal entries containing one factor of \( t \) each; all the corresponding terms are \( O(t^2) \). In the term in which \( \pi \) is the identity permutation, expand the product \( \prod_{i=1}^m (1 + t(A_0^{-1}B(t))_{ii}) \) to obtain \( 1 + t \sum_{i=1}^m (A_0^{-1}B(t))_{ii} + O(t^2) \). Thus

\[
\det A(t) = \det A_0 + t \det A_0 \tr(A_0^{-1}B(0)) + O(t^2), \tag{B.14}
\]

showing that \( \frac{d}{dt}|_{t=0} \det A(t) = \det A(0) \tr(A(0)^{-1}A'(0)) \). The point \( t = 0 \) plays no special role, so we can rearrange to obtain (B.10). Applying (B.10) to \( \log \hat{P} = -\frac{1}{2} \log \det(2\pi K''n) \),

\[
\frac{\partial}{\partial t} \log \hat{P}(\theta, s) = -\frac{1}{2} \tr \left( K''(s; \theta)^{-1} \frac{\partial K''}{\partial t}(s; \theta) \right). \tag{B.15}
\]

We will apply (B.15) with the scalar \( t \) being one of the coordinates \( \theta_i \) or \( s_j \).

## C Proof of Proposition 15 and Corollary 17

The proof of Proposition 15 is based on an asymptotic expansion of \( P_n(\theta, s) \) and its derivatives when \( n \) is large. We will need to justify the interchange of integration and differentiation in (4.6)–(4.7), and we state a sufficient condition in Lemma 19 below.

In addition, passing from the discrete parameter \( n \) to the continuous parameter \( \varepsilon \) will require us to define an analogue of (4.6) for non-integer \( n \). Some care is required because, away from the real axis, \( K_0(s + i\varphi) = \log M_0(s + i\varphi) \) may have branch cuts at zeros of \( M_0 \). These make no difference in (4.6) provided that \( n \) is an integer, because the combination \( \exp(nK_0(s + i\varphi)) \) can be unambiguously interpreted as \( M_0(s + i\varphi)^n \). We will circumvent this by modifying \( K_0 \) away from the real axis. This modification introduces error terms indexed by \( n \in \mathbb{N} \), which will prove to be negligible as \( n \to \infty \). We will use Lemmas 20–21 to show that these error terms can be extended to be indexed by \( \varepsilon \geq 0 \) in a continuously differentiable way.

**Lemma 19.** Let \( U \subset \mathbb{R}^{k \times 1} \) be open, let \( \mu \) be a measure on a space \( \mathcal{Y} \), let \( h(y) \geq 0 \) be a measurable function with \( \int h(y) \, d\mu(y) < \infty \), and let \( g(x, y) : U \times \mathcal{Y} \to \mathbb{R} \) be such that

\[
f(x) = \int_{\mathcal{Y}} g(x, y) \, d\mu(y) \tag{C.1}
\]

converges for all \( x \in U \).
Lemma 20. Let \( |g(x, y)| \leq h(y) \) for all \( x \in U \) and if \( g(\cdot, y) \) is continuous at \( x_0 \) for \( \mu \)-almost every \( y \), then \( f \) is continuous at \( x_0 \).

(b) Fix an entry \( x_i \) of \( x \) and suppose that \( g(x, y) \) is continuously differentiable as a function of \( x_i \), for all fixed values of \( y \) and \( x_j \), \( j \neq i \). Suppose in addition that \( \frac{\partial g}{\partial x_i}(x, y) \) is jointly measurable and \( \left| \frac{\partial g}{\partial x_i}(x, y) \right| \leq h(y) \) for all \( x \in U \). Then

\[
\frac{\partial f}{\partial x_i}(x) = \int_0^1 \frac{\partial g}{\partial x_i}(x, y) \, dy \quad (C.2)
\]

for all \( x \in U \).

(c) If in addition \( \frac{\partial f}{\partial x_i}(\cdot, y) \) is continuous at \( x_0 \) for \( \mu \)-almost every \( y \), then \( \frac{\partial f}{\partial x_i} \) is continuous at \( x_0 \).

Proof. For part (a), the integrand \( g(x, y) \) converges \( \mu \)-a.e. to \( g(x_0, y) \) as \( x \to x_0 \) and is bounded by the integrable function \( h \). So the Dominated Convergence Theorem gives the result.

For part (b), let \( e_i \) denote the unit vector in the \( i \)th coordinate direction. Then given \( x \in U \), we can write

\[
\frac{f(x + te_i) - f(x)}{t} = \int_Y \int_0^1 \frac{\partial g}{\partial x_i}(x + te_i, y) \, dy \, du \quad (C.3)
\]

for all \( t \neq 0 \) sufficiently small. The integrand in (C.3) is bounded by the integrable function \( h(y)1_{[0,1]}(u) \) and converges pointwise as \( t \to 0 \), so (C.2) follows by the Dominated Convergence Theorem.

Finally part (c) follows by applying part (a) to (C.2). \( \square \)

The next result explains when we can interpolate a given sequence by a continuously differentiable function. Here and elsewhere, continuous differentiability on a set with boundary points includes differentiability at the boundary (interpreting derivatives as one-sided derivatives as appropriate) and the derivatives are required to be continuous up to and including the boundary.

**Lemma 20.** Let \( \varepsilon_n \) be a sequence with \( 0 < \varepsilon_{n+1} < \varepsilon_n \in [0, 1] \) for all \( n \in \mathbb{N} \) and \( \varepsilon_n \to 0 \) as \( n \to \infty \), and let \( r_n \) be a real-valued sequence defined for \( n \in \mathbb{N} \), \( n \geq n_0 \). Then

\[
\lim_{n \to \infty} r_n = 0, \quad \lim_{n \to \infty} \frac{r_n - r_{n+1}}{\varepsilon_n - \varepsilon_{n+1}} = 0, \quad (C.4)
\]

is a necessary and sufficient condition for the existence of a continuously differentiable function \( f : [0, 1] \to \mathbb{R} \) satisfying \( f(0) = 0 \), \( f'(0) = 0 \) and \( f(\varepsilon_n) = a_n \) for all \( n \geq n_0 \).

Proof. For necessity, \( r_n \to 0 \) follows by taking \( f(\varepsilon) \to f(0) = 0 \) along \( \varepsilon = \varepsilon_n \). We can write

\[
\frac{r_n - r_{n+1}}{\varepsilon_n - \varepsilon_{n+1}} = \int_0^1 f'(u \varepsilon_n + (1-u) \varepsilon_{n+1}) \, du,
\]

and the integrand tends uniformly to \( f'(0) = 0 \) as \( n \to \infty \).

For sufficiency, fix a smooth function \( \eta : \mathbb{R} \to \mathbb{R} \) whose support is a compact subset of \((0, 1)\) and such that \( \int_0^1 \eta(u) \, du = 1 \). Define

\[
h(\varepsilon) = \sum_{n=n_0}^{\infty} \frac{r_n - r_{n+1}}{\varepsilon_n - \varepsilon_{n+1}} \eta \left( \frac{\varepsilon - \varepsilon_{n+1}}{\varepsilon_n - \varepsilon_{n+1}} \right), \quad f(\varepsilon) = \int_0^\varepsilon h(y) \, dy. \quad (C.5)
\]

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We claim that \( f \) has the required properties. Note that the \( n \)th term contributing to \( h(\varepsilon) \) is supported in \((\varepsilon_{n+1}, \varepsilon_n)\). Hence around each fixed \( \varepsilon > 0 \) there is a neighbourhood in which at most two summands contribute to \( h \), and it follows that \( h \) is continuous on \([0, 1]\). Moreover \( h(0) = 0 \), and \( \frac{r_n - r_{n+1}}{\varepsilon_n - \varepsilon_{n+1}} \to 0 \) as \( n \to \infty \) implies that \( h(\varepsilon) \to 0 \) as \( \varepsilon \to 0 \). (Here we have used the disjointness of the intervals \((\varepsilon_{n+1}, \varepsilon_n)\) and the boundedness of \( \eta \).) Thus \( h \) is continuous and bounded on \([0, 1]\), implying that \( f \) is continuously differentiable.

It remains to verify that \( f(\varepsilon_n) = a_n \) or equivalently that \( \int_0^{\varepsilon_n} h(\varepsilon) \, d\varepsilon = r_n \), for all \( n \geq n_0 \). By the choice of \( \eta, f^{\varepsilon_n} \), \( h(\varepsilon) \, d\varepsilon = r_n - r_{n+1} \), and a finite sum implies \( \int_0^{\varepsilon_n} h(\varepsilon) \, d\varepsilon = r_n - r_{N+1} \). Take \( N \to \infty \). The Dominated Convergence Theorem applies, so the integral converges to \( \int_0^{\varepsilon_n} h(\varepsilon) \, d\varepsilon \), while \( r_{N+1} \to 0 \) by assumption.

**Lemma 21.** Let \( \varepsilon_n \) be a sequence with \( 0 < \varepsilon_{n+1} < \varepsilon_n \in [0, 1] \) for all \( n \in \mathbb{N} \) and \( \varepsilon_n \to 0 \) as \( n \to \infty \). Let \( S \subset \mathbb{R}^k \) and let \( r_n : S_n \to \mathbb{R}, n \in \mathbb{N} \), be continuously differentiable functions defined on subsets \( S_n \subset S \). Suppose that for each \( x_0 \in \text{int} S \), there exists a neighbourhood \( G \subset S \) of \( x_0 \) and \( n_0 \in \mathbb{N} \) such that \( G \subset S_n \) for all \( n \geq n_0 \) and

\[
\lim_{n \to \infty} \sup_{x \in G} r_n(x) = 0.
\]

Then there exist a subset \( \mathcal{Q} \subset S \times [0, 1] \), open relative to \( S \times [0, 1] \) and containing \( \{(x, 0) : x \in \text{int} S \} \), and a continuously differentiable function \( f(x, \varepsilon) \) defined on \( \mathcal{Q} \), such that \( f(x, 0) = 0 \), \( \frac{\partial f}{\partial \varepsilon}(x, 0) = 0 \) and \( f(x, \varepsilon_n) = r_n(x) \) whenever \((x, \varepsilon_n) \in \mathcal{Q}\).

**Proof.** Let \( \tilde{r}_n(x) \) be a continuously differentiable function defined on \( \mathbb{R}^k \) that agrees with \( r_n(x) \) on \( \{x : d(x, S_n^c) \geq 1/n\} \). Such a function can be constructed by, for instance, taking an infinitely differentiable function \( \eta(t) \) with \( \eta(t) = 1 \) if \( t \geq 1/n \) and \( \eta(t) = 0 \) if \( t \leq 1/2n \), and setting \( \tilde{r}_n(x) = r_n(x) \eta(n d(x, S_n^c)) \).

Let \( x_0 \in \text{int} S \) with the corresponding neighbourhood \( G \) and \( n_0 \in \mathbb{N} \). We can choose an open ball \( \bar{G}_{x_0} \subset G \) containing \( x_0 \) and \( n_1 \in \mathbb{N} \) such that every \( x \in \bar{G}_{x_0} \) satisfies \( d(x, G^c) \geq 1/n_1 \). Write \( \tilde{n}(x_0) = \max\{n_0, n_1\} \). Then, for all \( n \geq \tilde{n}(x_0) \), \( r_n \) is defined on \( \bar{G}_{x_0} \) and agrees with \( \tilde{r}_n \) there. In particular, (C.6) remains true when we replace \( r_n, r_{n+1} \) and \( G \) by \( \tilde{r}_n, \tilde{r}_{n+1} \) and \( \bar{G}_{x_0} \).

For each \( x_0 \in \text{int} S \), apply Lemma 20 with \( r_n \) replaced by \( \tilde{r}_n(x_0) \), noting that the assumptions apply because of (C.6), to produce functions \( \varepsilon \mapsto f(x_0, \varepsilon) \) and \( \varepsilon \mapsto h(x_0, \varepsilon) \). By construction, \( f(x_0, 0) = 0 \) and \( \frac{\partial f}{\partial \varepsilon}(x_0, 0) = 0 \). Moreover \( f(x_0, \varepsilon_n) = \tilde{r}_n(x_0) \) for all \( n \in \mathbb{N} \), and therefore \( f(x, \varepsilon_n) = r_n(x) \) for all \( x \in \bar{G}_{x_0} \) and \( n \geq \tilde{n}(x_0) \). Thus if we set \( \mathcal{Q} = \bigcup_{x \in \text{int} S} \bar{G}_x \times [0, \varepsilon_{\tilde{n}(x)}] \) then \( f(x, \varepsilon_n) = r_n(x) \) whenever \( (x, \varepsilon_n) \in \mathcal{Q} \), as required.

It remains to show that \( f \) is continuously differentiable. By construction, \( \frac{\partial f}{\partial \varepsilon}(x, \varepsilon) = h(x, \varepsilon) \), so it suffices to show that \( h \) and \( \nabla_x f \) are continuous as functions of both variables. Note that the partial sums of the series that define \( h(x, \varepsilon) \) are continuously differentiable. By the same argument as in the proof of Lemma 20, it follows that \( h \) and \( \nabla_x h \) are both continuous for \( \varepsilon > 0, x \in U \), and \( \nabla_x h(x, \varepsilon) = \sum_{n=n_0}^{\infty} \frac{\nabla_x r_n(x) - \nabla_x r_{n+1}(x)}{\varepsilon_n - \varepsilon_{n+1}} \eta(\varepsilon - \varepsilon_{n+1}) \) for all \( \varepsilon > 0 \). Since \( h(x, 0) \) is identically zero we have \( \nabla_x h(x, 0) = 0 \). By the assumptions, both \( h(x, \varepsilon) \) and \( \nabla_x h(x, \varepsilon) \) converge to 0 as \( \varepsilon \to 0 \), uniformly in \( x \), so it follows that \( h \) and \( \nabla_x h \) are also continuous (as functions of two variables) at \( \varepsilon = 0, x \in U \). Finally Lemma 19 implies that

\[
\nabla_x f(x, \varepsilon) = \int_0^\varepsilon \nabla_x h(x, y) \, dy = \int_0^1 \nabla_x h(x, y) 1_{\{y \leq \varepsilon\}} \, dy.
\]

(C.7)
Since $\mathbb{1}_{\{y \leq \varepsilon\}}$ is continuous at $\varepsilon_0$ for almost all $y$, a further application of Lemma 19 implies that $\nabla_x f$ is continuous.

We are now ready to prove Proposition 15.

**Proof of Proposition 15.** We first claim that we can find a continuous function $\delta(s, \theta)$ defined on $\mathcal{S}$ such that for all $(s, \theta) \in \mathcal{S}$,

$$\text{Re} \ M_0(s + i\varphi; \theta) > \delta(s, \theta) \quad \text{for all } \varphi \in \mathbb{R}^{1 \times m} \text{ with } |\varphi| \leq 2\delta(s, \theta)$$

(C.8)

and

$$v \text{Re} \ K''_0(s + i\varphi; \theta)v^T \geq \delta(s, \theta) |v|^2 \quad \text{for all } v, \varphi \in \mathbb{R}^{1 \times m} \text{ with } |\varphi| \leq 2\delta(s, \theta),$$

(C.9)

as well as the bounds (2.12)–(2.13). In particular, we can locally define $K_0(s + i\varphi; \theta) = \log M_0(s + i\varphi; \theta)$ for $|\varphi| \leq 2\delta(s, \theta)$, where $\log$ denotes the standard branch of the logarithm with a branch cut along the negative real axis. (Note that we did not need to specify this choice of branch cut for the logarithm in order to state (C.9) because $K'_0(s + i\varphi; \theta)$ is given unambiguously as $K'_0 = M'_0/M_0$ in all cases.) The function $K_0$ thus defined has the same smoothness properties as $M_0$.

For (C.8), the Mean Value Theorem and (2.13) with $k = 0, \ell = 1$ show that if $|\varphi| \leq \min \{M_0(s; \theta)/4\gamma(s, \theta)3^{\gamma(s, \theta)}, 1\}$ then $\text{Re} \ M_0(s + i\varphi; \theta) \geq \frac{1}{2} M_0(s; \theta)$. In all of the assertions, we are free to replace $\delta(s, \theta)$ by a smaller positive quantity, so the first part of the claim follows by replacing the function $\delta(s, \theta)$ from (2.12)–(2.13) by

$$\min \{\delta(s, \theta), M_0(s; \theta)/4\gamma(s, \theta)3^{\gamma(s, \theta)}, 1, \frac{1}{2} M_0(s; \theta)\}.$$

(C.10)

The bound (C.9) follows by a similar argument using (2.13) with $k = 0$ and $\ell \in \{1, 2, 3\}$.

Fix an infinitely differentiable function $\eta(s, \theta, \varphi)$ with values in $[0, 1]$ and satisfying $\eta(s, \theta, \varphi) = 0$ if $|\varphi| \geq 2\delta(s, \theta)$ and $\eta(s, \theta, \varphi) = 1$ if $|\varphi| \leq 1$. We may assume moreover that $\varphi \mapsto \eta(s, \theta, \varphi)$ is radially symmetric for each fixed $(s, \theta) \in \mathcal{S}$. (For instance, we may find an infinitely differentiable function $\bar{\delta}(s, \theta)$ such that $\frac{2}{3}\delta(s, \theta) \leq \bar{\delta}(s, \theta) \leq \delta(s, \theta)$. Then set $\eta(s, \theta, \varphi) = \tilde{\eta}(|\varphi|/\bar{\delta}(s, \theta))$ where $\tilde{\eta}$ is infinitely differentiable with $\tilde{\eta}(r) = 0$ for $r \geq 2$ and $\tilde{\eta}(r) = 1$ for $r \leq \frac{3}{2}$.) In addition, all derivatives of $\eta$ are supported in the region $\delta(s, \theta) \leq |\varphi| \leq 2\delta(s, \theta)$.

In the rest of the proof, we will construct the functions $q_1, q_2$. In order to show continuous differentiability, we will focus our attention on a fixed but arbitrary point $(s_0, \theta_0) \in \text{int} \ \mathcal{S}$, and suitable chosen neighbourhoods $U$ of $\theta_0$ and $W$ of $s_0$. This will not entail any loss of generality because continuous differentiability is a local property, while, as we shall see, the construction of $q_1, q_2$ does not depend on the choice of $(s_0, \theta_0), U$ or $W$.

Let $(s_0, \theta_0) \in \text{int} \ \mathcal{S}$ be given. Since $\delta(s, \theta)$ and $\gamma(s, \theta)$ are continuous, we may choose neighbourhoods $U, W$ and constants $\delta_0 > 0, \gamma_0 < \infty$ such that

$$\delta(s, \theta) \geq \delta_0, \quad \gamma(s, \theta) \leq \gamma_0 \quad \text{for all } s \in W, \theta \in U.$$  

(C.11)

The numbers $\delta_0, \gamma_0$ and the neighbourhoods $U, W$ will now be fixed for the remainder of the proof. We remark that the bounds (2.12)–(2.13) and (C.8)–(C.9) are monotone in $\delta$ and $\gamma$, so they hold uniformly over $U, W$ with $\delta(s, \theta), \gamma(s, \theta)$ replaced by $\delta_0, \gamma_0$. 

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Recall that $K_0(s + i\varphi)$ can be defined for $|\varphi| \leq 2\delta(s, \theta)$, but may not be defined globally. We will therefore rewrite the integrals in (4.6)–(4.7) by defining

$$w(s, \varphi, \theta) = \frac{M_0(s + i\varphi; \theta)e^{-i\varphi K_0'(s; \theta)}}{M_0(s)},$$

$$I_1(\theta, s, n) = \int_{\mathbb{R}^1 \times m} w(s, \varphi, \theta)^n \frac{d\varphi}{(2\pi)^m},$$

$$I_2(\theta, s, n) = \int_{\mathbb{R}^1 \times m} w(s, \varphi, \theta)^{n-1} \frac{\partial w}{\partial t}(s, \varphi, \theta) \frac{d\varphi}{(2\pi)^m}.$$  \hfill (C.12)

Let $\tau$ denote another entry $\theta_i$ or $s_j$ (possibly the same entry as $t$) and define

$$I_3 = \int_{\mathbb{R}^1 \times m} w(s, \varphi, \theta)^{n-2} \left[ n(n-1) \frac{\partial w}{\partial \tau}(s, \varphi, \theta) \frac{\partial w}{\partial t}(s, \varphi, \theta) + n \frac{\partial^2 w}{\partial \tau \partial t}(s, \varphi, \theta) \right] \frac{d\varphi}{(2\pi)^m}.$$  \hfill (C.13)

Thus the integrands for $I_2, I_3$ are $\frac{\partial}{\partial \gamma}$ and $\frac{\partial^2}{\partial \gamma \partial t}$ of the integrand for $I_1$. Throughout the proof we will think of $t$ and $\tau$ as fixed but arbitrary; thus our conclusions about $I_2$ will apply mutatis mutandis to the integral with $\frac{\partial w}{\partial \tau}$ replaced by $\frac{\partial w}{\partial \gamma}$.

It is readily verified that $\frac{\partial w}{\partial \tau}$ and $\frac{\partial^2 w}{\partial \tau \partial t}$ can be expressed as multivariate polynomials in the arguments $\varphi$, $M_0(s + i\varphi)/M_0(s)$, $\frac{\partial M_0}{\partial \tau}(s + i\varphi)$, and $\frac{\partial^2 M_0}{\partial \tau \partial t}(s + i\varphi)$; the same quantities evaluated at $\varphi = 0$; $\frac{\partial M_0'}{\partial \tau}(s)$, $\frac{\partial M_0'}{\partial \tau}(s)$ and $\frac{\partial^2 M_0'}{\partial \tau \partial t}(s)$; and $1/M_0(s)$. By (2.13), it follows that

$$\max \{ |\frac{\partial w}{\partial \tau}|, |\frac{\partial w}{\partial \gamma}|, |\frac{\partial^2 w}{\partial \tau \partial t}| \} \leq C(1 + |\varphi|)^\alpha$$

for some $C, \alpha < \infty$ that depend only on $\delta_0, \gamma_0$. On the other hand, (2.12) implies

$$|w(s, \varphi, \theta)| \leq (1 + \delta_0 |\varphi|^2)^{-\delta_0}$$

since the upper bound in (2.12) is monotone in $\delta$. So the integrands in (C.12)–(C.13) can be bounded by

$$n^2(C^2 + C + 1)(1 + |\varphi|)^{\alpha} (1 + \delta_0 |\varphi|^2)^{-\delta_0(n-2)}$$

uniformly in $\theta, s$, and the function in (C.16) is integrable (for fixed $n$) as soon as $2\delta_0(n - 2) - 2\alpha > m$. Thus if we define $n_0 = 3 + (m + 2\alpha)/2\delta_0$ then the integrands in (C.12)–(C.13) are dominated by integrable functions for each $n \geq n_0$. In particular, by Lemma 19, for all $n \geq n_0$,

$$I_1(\theta, s, n) = P_n(\theta, s), \quad I_2 = \frac{\partial I_1}{\partial t} = \frac{\partial P_n}{\partial t}, \quad I_3 = \frac{\partial I_2}{\partial \tau}.$$  \hfill (C.17)

with $I_1, I_2, I_3$ continuous for fixed $n$.

Define

$$h(s, \varphi, \theta) = \eta(s, \theta, \varphi) \left[ K_0(s + i\varphi; \theta) - K_0(s; \theta) - i\varphi K_0'(s; \theta) \right] + (1 - \eta(s, \theta, \varphi)) \left[ -\frac{1}{2} \varphi K''_0(s; \theta) \varphi^T \right].$$  \hfill (C.18)

Note that $h$ is well-defined since by construction $\eta$ is supported in the region where $K_0$ is well-defined. We remark that $h$ behaves quadratically in $\varphi$ for $|\varphi|$ small. To emphasise this, apply Lagrange’s form of the remainder term,

$$f(1) - f(0) - f'(0) = \int_0^1 (1-u)f''(u) \ du,$$

(19)
with the function

\[ f(u) = \eta(s, \theta, \varphi)K_0(s + iu \varphi) - \frac{1}{2} u^2 (1 - \eta(s, \theta, \varphi)) \varphi K''_0(s) \varphi^T. \]  

(20)

Thus, writing

\[ g(s, \varphi, \theta, u) = \eta(s, \theta, \varphi)K''_0(s + iu \varphi; \theta) + (1 - \eta(s, \theta, \varphi))K''_0(s), \]  

(21)

we can rewrite \( h \) as

\[ h(s, \varphi, \theta) = -\int_0^1 (1 - u) \varphi g(s, \varphi, \theta, u) \varphi^T \, du. \]  

(22)

Then (C.9) implies

\[ v \Re g(s, \varphi, \theta, u) v^T \geq \delta_0 |v|^2, \quad \Re h(s, \varphi, \theta) \leq -\frac{1}{2} \delta_0 |\varphi|^2. \]  

(23)

Since \( K''_0 = M''_0/M_0 - (M_0''/M_0)^2 \), the partial derivatives \( \frac{\partial}{\partial t}, \frac{\partial}{\partial \tau} \) and \( \frac{\partial^2}{\partial \tau \partial t^2} \) can be expressed as multivariate polynomials in the arguments \( \frac{\partial M_0}{\partial \tau} (s + iu \varphi), \frac{\partial M_0}{\partial t} (s + iu \varphi), \frac{\partial^2 M_0}{\partial \tau \partial t} (s + iu \varphi), \frac{\partial M_0''}{\partial \tau} (s + iu \varphi), \frac{\partial M_0''}{\partial t} (s + iu \varphi), \frac{\partial^2 M_0''}{\partial \tau \partial t} (s + iu \varphi), \) and \( 1/M_0(s + iu \varphi) \); the same quantities evaluated at \( \varphi = 0 \); and \( \eta(s, \theta, \varphi) \) and its derivatives. Note that \( 1/M_0(s + iu \varphi) \) may become unbounded if \( M_0 \) has zeros, but powers \( 1/M_0(s + iu \varphi)^k \) only appear in combination with a factor \( \eta(s, \theta, \varphi) \) or one of its derivatives, all of which are supported in the region \( |\varphi| \leq 2\delta(s, \theta) \) where (C.8) applies. It follows that each such combination is uniformly bounded. Hence, by (2.13), \( g \) and its partial derivatives (and hence, by Lemma 19, \( h \) and its partial derivatives) grow at most polynomially in \( \varphi \):

\[ \max \left\{ \left| \frac{\partial g}{\partial t} \right|, \left| \frac{\partial g}{\partial \tau} \right|, \left| \frac{\partial^2 g}{\partial \tau \partial t} \right|, \left| \frac{\partial^2 g}{\partial \tau^2} \right|, \left| \frac{\partial^2 g}{\partial \tau \partial t^2} \right| \right\} \leq C''(1 + |\varphi|)^\alpha' \]  

(24)

for some \( C'', \alpha' < \infty \) that depend only on \( \delta_0, \gamma_0 \). The same argument (involving up to 3 \( s \)-derivatives of \( M''_0 \) and \( \frac{\partial M''_0}{\partial t} \)) shows that

\[ \max \left\{ \left| \frac{\partial^2 g}{\partial \tau \partial t} \right|, \left| \frac{\partial^2 g}{\partial \tau^2} \right|, \left| \frac{\partial^3 g}{\partial \tau \partial t^2} \right|, \left| \frac{\partial^3 g}{\partial \tau \partial t \partial \tau} \right|, \left| \frac{\partial^3 g}{\partial \tau^2 \partial t} \right|, \left| \frac{\partial^3 g}{\partial \tau^3} \right| \right\} \leq C''(1 + |\varphi|)^\alpha'' \]  

(25)

for some \( C'', \alpha'' < \infty \) that also depend only on \( \delta_0, \gamma_0 \).

By analogy with (C.12)–(C.13), define

\[ J_1(\theta, s, \varepsilon) = \int_{\mathbb{R}^{1 \times m}} \exp \left( \varepsilon^{-1} h(s, \varphi, \theta) \right) \frac{d\varphi}{(2\pi)^m}; \]

\[ J_2(\theta, s, \varepsilon) = \int_{\mathbb{R}^{1 \times m}} \exp \left( \varepsilon^{-1} h(s, \varphi, \theta) \right) \varepsilon^{-1} \frac{\partial h}{\partial t}(s, \varphi, \theta) \frac{d\varphi}{(2\pi)^m}, \]

\[ J_3(\theta, s, \varepsilon) = \int_{\mathbb{R}^{1 \times m}} \exp \left( \varepsilon^{-1} h(s, \varphi, \theta) \right) \left[ \varepsilon^{-1} \frac{\partial^2 h}{\partial t^2}(s, \varphi, \theta) + \varepsilon^{-2} \frac{\partial h}{\partial t}(s, \varphi, \theta) \frac{\partial h}{\partial t}(s, \varphi, \theta) \right] \frac{d\varphi}{(2\pi)^m}. \]  

(26)

The bounds (C.23)–(C.24) imply that the integrands in (26) can be bounded by

\[ \varepsilon^{-2}((C')^2 + C' + 1)(1 + |\varphi|)^{2\alpha' \exp \left( -\frac{1}{2} \delta_0 |\varphi|^2 \right)} \]  

(27)
Furthermore \( \varepsilon > 0 \) in (C.26) and use (C.22):

\[
J_2 = \frac{\partial J_1}{\partial t}, \quad J_3 = \frac{\partial J_2}{\partial \tau} \quad \text{for all } \varepsilon > 0.
\]

(C.28)

Furthermore \( J_1, J_2, J_3 \) are continuous in all three variables in the region \( \varepsilon > 0 \).

We will next show that, for \( k = 1, 2, 3 \),

\[
r_n^{(k)}(\theta, s) = \frac{I_k(\theta, s, n) - J_k(\theta, s, 1/n)}{P_n(\theta, s)}
\]

(C.29)

satisfies \( r_n^{(k)}(\theta, s) = o(n^{-2}) \) uniformly over \( \theta \in U, s \in W \). Note that the integrands defining \( I_k(\theta, s, n) \) and \( J_k(\theta, s, 1/n) \) agree over the region \( |\varphi| \leq \delta_0 \) because \( \eta(s, \theta, \varphi) = 1 \) and \( \exp(h) = w \) there. When \( n \geq n_0 \) and \( |\varphi| \geq \delta_0 \), the quantities in (C.16) and (C.27) (with \( \varepsilon^{-1} \) replaced by \( n \)) are bounded by

\[
C^n(1 + |\varphi|)^{2a'n'} \left( (1 + \delta_0 |\varphi|)^{-\delta_0(n-0-2)} + \exp(\frac{1}{2} n_0 \delta_0 |\varphi|^2) \right)
\]

\[
\cdot n^2 \left( (1 + \delta_0)^{-\delta_0(n-n_0)} + \exp(\frac{1}{2}(n - n_0)\delta_0^2) \right)
\]

uniformly in \( \theta, s \). Integrating over \( \varphi \) leads to the conclusion that \( I_k(\theta, s, n) - J_k(\theta, s, 1/n) \) decays exponentially in \( n \), uniformly in \( \theta, s \). Since \( P_n(\theta, s)^{-1} = O(n^{m/2}) \), uniformly in \( \theta, s \), we have

\[
r_n^{(k)}(\theta, s) = o(n^{-2}) \quad \text{uniformly over } \theta \in U, s \in W,
\]

(C.31)
as asserted.

Next we apply Lemma 21 to \( r_n^{(k)}(\theta, s) \) for \( k = 1, 2 \). We set \( \varepsilon_n = 1/n \), so that \( \varepsilon_n - \varepsilon_{n+1} \sim n^{-2} \). Recalling (C.17) and (C.28), the identity

\[
\frac{\partial}{\partial \tau} \left( \frac{Z}{P_n(\theta, s)} \right) = \frac{\partial Z}{\partial \tau} \frac{Z}{P_n(\theta, s)} \frac{\partial}{\partial \tau} \log \hat{P}(\theta, s)
\]

(C.32)

with \( Z = I_k - J_k \) allows us to express the gradients \( \nabla \theta r_n^{(k)} \) and \( \nabla_s r_n^{(k)} \) for \( k = 1, 2 \) in terms of \( r_n^{(2)} \) (or rather, the analogue of \( r_n^{(2)} \) with \( t \) replaced by \( \tau \)) and \( r_n^{(3)} \). Since \( \frac{\partial}{\partial \tau} \log \hat{P}(\theta, s) \) is bounded and continuous in \( \theta, s \), and does not depend on \( n \), it follows that \( \nabla \theta r_n^{(k)} \) and \( \nabla_s r_n^{(k)} \) are continuous and \( o(n^{-2}) \), uniformly in \( \theta, s \), for \( k = 1, 2 \). By Lemma 21 we can find continuously differentiable functions \( \tilde{f}_1(\theta, s, \varepsilon), \tilde{f}_2(\theta, s, \varepsilon) \) such that

\[
\tilde{f}_1(\theta, s, 1/n) = \frac{P_n(\theta, s) - J_1(\theta, s, 1/n)}{P_n(\theta, s)}, \quad \tilde{f}_2(\theta, s, 1/n) = \frac{\partial P_n(\theta, s) - J_2(\theta, s, 1/n)}{P_n(\theta, s)}
\]

(C.33)

for \( \theta \in U, s \in W, n \geq n_0 \).

We claim that \( J_k(\theta, s, 1/n)/P_n(\theta, s) \), \( k = 1, 2 \), can be extended to be continuously differentiable functions of \( \theta, s, \varepsilon = 1/n \), including at \( \varepsilon = 0 \). We have already defined \( J_k \) for all \( \varepsilon > 0 \), and we can extend \( P_n(\theta, s) \) by declaring that (4.5) holds whether or not \( n > 0 \) is an integer. To handle the extension to \( \varepsilon = 0 \), substitute \( \varphi = \psi \sqrt{\varepsilon} \), \( d\varphi = \varepsilon^{m/2} d\psi \) in (C.26) and use (C.22):

\[
\int_{\mathbb{R}^{1\times m}} \exp \left( \varepsilon^{-1} h(s, \varphi, \theta) \right) \frac{\sqrt{\det(2\pi K_0(s, \theta))}}{(2\pi)^m \varepsilon^{m/2}} d\varphi = \int_{\mathbb{R}^{1\times m}} \exp \left( - \int_0^1 (1 - u) \psi \sqrt{\varepsilon} \psi^T d\psi \right) \frac{\sqrt{\det(2\pi K_0(s, \theta)^{-1})}}{(2\pi)^m \varepsilon^{m/2}} d\psi.
\]

(C.34)
Similar considerations hold for $J_2$ and $J_3$. Define

$$f_1(\theta, s, \varepsilon) = \int_{\mathbb{R}^1 \times m} \frac{\exp\left(-\int_0^1 (1-u)\psi g(s, \psi \sqrt{\varepsilon}, \theta, u)\psi^T du\right)}{\sqrt{\det(2\pi K_0''(s; \theta))}} \, d\psi,$$

$$f_2(\theta, s, \varepsilon) = \int_{\mathbb{R}^1 \times m} \frac{\exp\left(-\int_0^1 (1-u)\psi g(s, \psi \sqrt{\varepsilon}, \theta, u)\psi^T du\right)}{\sqrt{\det(2\pi K_0''(s; \theta))}} \cdot \left(-\int_0^1 (1-u)\psi \frac{\partial g}{\partial t}(s, \psi \sqrt{\varepsilon}, \theta, u)\psi^T du\right) \, d\psi,$$

$$f_3(\theta, s, \varepsilon) = \int_{\mathbb{R}^1 \times m} \frac{\exp\left(-\int_0^1 (1-u)\psi g(s, \psi \sqrt{\varepsilon}, \theta, u)\psi^T du\right)}{\sqrt{\det(2\pi K_0''(s; \theta))}} \cdot \left(\int_0^1 (1-v)\psi \frac{\partial g}{\partial \tau}(s, \psi \sqrt{\varepsilon}, \theta, v)\psi^T dv \int_0^1 (1-u)\psi \frac{\partial g}{\partial t}(s, \psi \sqrt{\varepsilon}, \theta, u)\psi^T du \right. \right.$$

$$\left. - \int_0^1 (1-u)\psi \frac{\partial^2 g}{\partial \tau \partial t}(s, \psi \sqrt{\varepsilon}, \theta, u)\psi^T du \right) \, d\psi \tag{C.35}$$

for $\varepsilon \geq 0$. Lemma 19 applied repeatedly to (C.22) confirms that

$$f_k(\theta, s, \varepsilon) = \frac{J_k(\theta, s, \varepsilon)}{P_{1/e}(\theta, s)} \tag{C.36}$$

for all $\varepsilon > 0$. The integrands in (C.35) are continuous in all of their variables, including at $\varepsilon = 0$, and by (C.23)–(C.24) are bounded by

$$((C')^2 + C' + 1)(1 + |\psi|^2)^{2a'+2} \exp\left(-\frac{1}{2}\delta_0 |\psi|^2\right) \tag{C.37}$$

for all $\varepsilon \in [0, 1]$. The function in (C.37) is integrable, so Lemma 19 implies that $f_1, f_2, f_3$ are continuous. By another application of (C.32) with $Z = f_k$, $k = 1, 2$, the continuity of $f_2, f_3$ implies that $\frac{\partial f_1}{\partial \varepsilon}, \frac{\partial f_2}{\partial \varepsilon}$ are continuous.

To complete the claim that $f_1, f_2$ are continuously differentiable, it suffices to show that $\frac{\partial f_1}{\partial \varepsilon}$ and $\frac{\partial f_2}{\partial \varepsilon}$ are continuous. This is less clear: the integrands in (C.35) are typically not differentiable at $\varepsilon = 0$ because of the $\sqrt{\varepsilon}$. However, in a Taylor expansion, the $\sqrt{\varepsilon}$ term is odd as a function of $\psi$ and therefore makes no contribution to the integral. To see this, note that the integrands defining $f_1, f_2$ can be written in the form $H_k(\psi, \psi \sqrt{\varepsilon})$, where

$$H_1(v, \varphi) = \frac{\exp\left(-\int_0^1 (1-u)v g(s, \varphi, \theta, u)v^T du\right)}{\sqrt{\det(2\pi K_0''(s; \theta))}}, \tag{C.38}$$

$$H_2(v, \varphi) = -H_1(v, \varphi) \int_0^1 (1-u)v \frac{\partial g}{\partial t}(s, \varphi, \theta, u)v^T du.$$

(For convenience we omit the dependence on $\theta, s$.) Apply (C.19) with $f(u) = H_k(v, u \varphi)$ to find

$$H_k(\psi, \psi \sqrt{\varepsilon}) = H_k(\psi, 0) + \sqrt{\varepsilon} \psi \nabla_\varphi H_k(\psi, 0) + \varepsilon \int_0^1 (1-u)\psi \nabla_\varphi \nabla_\psi H_k(\psi, u \psi \sqrt{\varepsilon}) \psi^T du. \tag{C.39}$$

The quantities $H_k(v, \varphi)$ are even as functions of $v$ for each fixed $\varphi$, so that $\nabla_\varphi H_k(v, \varphi)$ is also even as a function of $v$. Hence $\psi \nabla_\varphi H_k(\psi, 0)$ is odd as a function of $\psi$. From
(C.23) and (C.25) it is straightforward to verify that \( H_k(v, \varphi), \frac{\partial H_k}{\partial \varphi_i}(v, \varphi), \frac{\partial^2 H_k}{\partial \varphi_i \varphi_j}(v, \varphi), \) for \( k = 1, 2 \) and \( i, j, \ell = 1, \ldots, m \), can all be bounded by

\[
C''''(1 + |\varphi| + |v|)^{s''''} \exp \left(-\frac{1}{2} \delta_0 |v|^2 \right)
\]  

(C.40)

for some constants \( C'''' \), \( \alpha'''' \) depending only on \( \delta_0, \gamma_0 \). In particular, the term \( \psi \nabla_\varphi H_k(\psi, 0) \) is integrable, so that oddness implies that its integral is zero. Thus

\[
f_k(\theta, s, \varepsilon) = \int_{\mathbb{R}^{1 \times m}} \left( H_k(\psi, 0) + \varepsilon \int_0^1 (1 - u) \psi \nabla_\varphi H_k^T(\psi, u \psi \sqrt{\varepsilon}) \psi^T du \right) d\psi.
\]  

(C.41)

In (C.41), the integrand is now continuously differentiable even at \( \varepsilon = 0 \), and (C.40) implies that its derivative with respect to \( \varepsilon \) is bounded by an integrable function. Thus Lemma 19 applies and verifies that \( f_1, f_2 \) are continuously differentiable.

Finally define \( q_k(\theta, s, \varepsilon) = f_k(\theta, s, \varepsilon) + f_k(\theta, s, \varepsilon) - f_k(\theta, s, 0) \) for \( \varepsilon \in [0, 1/n_0] \), so that \( q_1, q_2 \) are continuously differentiable and \( q_k(\theta, s, 0) = 0 \) by construction. Combining (C.33) and (C.36),

\[
\begin{align*}
\frac{P_n(\theta, s)}{P_n(\theta, s)} &= \frac{I_1(\theta, s, n)}{I_1(\theta, s, 1)} = \tilde{f}_1(\theta, s, 1/n) + f_1(\theta, s, 1/n) = f_1(\theta, s, 0) + q_1(\theta, s, 1/n), \\
\frac{\partial P_n(\theta, s)}{\partial s} &= \frac{I_2(\theta, s, n)}{I_2(\theta, s, 1)} = \tilde{f}_2(\theta, s, 1/n) + f_2(\theta, s, 1/n) = f_2(\theta, s, 0) + q_2(\theta, s, 1/n).
\end{align*}
\]  

(C.42)

We need to extend \( q_k \) to be defined for \( \varepsilon \in [-1/n_0, 1/n_0] \) (this is for convenience only, since the Implicit Function Theorem typically assumes that the base point belongs to the interior of the domain) and this can be done arbitrarily as long as \( q_k \) remains continuously differentiable. Since \( q_k(\theta, s, 0) \) vanishes identically, one way to make this extension is to require \( q_k \) to be an odd function of \( \varepsilon \). Lastly (4.8) follows from (C.42) by noting \( g(s, 0, \theta, u) = K_0''(s; \theta), \frac{\partial q}{\partial \varepsilon}(s, 0, \theta, u) = \frac{\partial K_0''}{\partial \varepsilon}(s; \theta) \) and calculating the Gaussian integrals

\[
\begin{align*}
f_1(\theta, s, \varepsilon) &= \int_{\mathbb{R}^{1 \times m}} \exp \left(-\frac{1}{2} \psi K_0''(s; \theta) \psi^T du \right) \sqrt{\det(2\pi K_0''(s; \theta)^{-1})} d\psi
= 1, \\
f_2(\theta, s, \varepsilon) &= -\int_{\mathbb{R}^{1 \times m}} \exp \left(-\frac{1}{2} \psi K_0''(s; \theta) \psi^T du \right) \sqrt{\det(2\pi K_0''(s; \theta)^{-1})} \frac{1}{2} \psi^T \frac{\partial K_0''}{\partial \psi}(s, \varphi) d\psi
= -\frac{1}{2} \text{tr} \left(K_0''(s; \theta)^{-1} \frac{\partial K_0''}{\partial \psi}(s, \varphi) \right)
= \frac{\partial}{\partial t} \log \hat{P}(\theta, s).
\end{align*}
\]

To prove Corollary 17, we first state an intermediate result.

**Corollary 22.** Under the hypotheses of Theorem 1, there are continuously differentiable functions \( q_5(\theta, s, \varepsilon), q_6(\theta, s, \varepsilon) \), with values in \( \mathbb{R}^{1 \times p} \) and \( \mathbb{R}^{m \times 1} \) respectively, defined on an open set \( \mathcal{Q}' \) containing \( \{(\theta, s, 0) : (s, \theta) \in \text{int} \mathcal{S} \} \), such that \( q_5(\theta, s, 0) = 0, q_6(\theta, s, 0) = 0 \) and

\[
\begin{align*}
\nabla_\theta \log P_n(\theta, s) &= \nabla_\theta \log \hat{P}(\theta, s) + q_5(\theta, s, 1/n), \\
\nabla_s \log P_n(\theta, s) &= \nabla_s \log \hat{P}(\theta, s) + q_6(\theta, s, 1/n)
\end{align*}
\]  

(C.43)

whenever \( (\theta, s, 1/n) \in \mathcal{Q}' \).
Proof. Let \( t \) denote one of the entries \( \theta_i \) or \( s_j \) and consider \( \frac{\partial}{\partial t} \log P_n(\theta, s) \). Comparing with the ratio of the two quantities in (4.8), set
\[
q_t(\theta, s, \varepsilon) = \frac{\frac{\partial}{\partial t} \log \hat{P}(\theta, s) + q_2(\theta, s, \varepsilon)}{1 + q_1(\theta, s, \varepsilon)} - \frac{\partial}{\partial t} \log \hat{P}(\theta, s) \\
= \frac{q_2(\theta, s, \varepsilon) - q_1(\theta, s, \varepsilon) \frac{\partial}{\partial t} \log \hat{P}(\theta, s)}{1 + q_1(\theta, s, \varepsilon)}.
\] (C.44)

We have immediately that \( q_t(\theta, s, 0) = 0 \). By Proposition 15 and (4.4), \( q_1 \) and \( q_2 \) are continuously differentiable, so \( q_t \) will be as well provided that \( q_1(\theta, s, \varepsilon) \neq -1 \). Since \( q_1(\theta, s, 0) = 0 \) and \( q_1 \) is continuous, we can rule out \( q_1(\theta, s, \varepsilon) = -1 \) by shrinking \( Q' \) to be a suitable subset of \( Q \). The functions \( q_5, q_6 \) are obtained by performing this construction \( p + m \) times, for each of the entries of \( \theta \) and \( s \).

Proof of Corollary 17. From (B.3) we have
\[
\nabla_{\theta} \left( \log P_n(\theta, \hat{s}_0(\theta; y)) \right) = \left( \nabla_{\theta} \log P_n \right)(\theta, \hat{s}_0(\theta; y)) + \left[ \left( \nabla_{s} \log P_n \right)(\theta, \hat{s}_0(\theta; y)) \right] \nabla_{\theta} \hat{s}_0^T(\theta; y),
\] (C.45)

so that if we set
\[
q_3(\theta, y, \varepsilon) = q_5(\theta, \hat{s}_0(\theta; y), \varepsilon) + q_6(\theta, \hat{s}_0(\theta; y), \varepsilon)^T \nabla_{\theta} \hat{s}_0^T(\theta; y)
\] (C.46)

then the relation (4.9) holds. The continuous differentiability of \( q_3 \) and the relation \( q_3(\theta, y, 0) = 0 \) follow from the corresponding properties for \( q_5, q_6 \) from Corollary 22 and the fact that \( \nabla_{\theta} \hat{s}_0^T \) is continuously differentiable, see (4.4).

D Proofs of Proposition 16 and Theorem 5

The proof of Proposition 16 is almost identical to that of Proposition 15, and we outline where and how they differ.

Proof of Proposition 16. The local bounds (C.8)–(C.9) use only (2.7) and (2.13), so they continue to hold (after possibly decreasing \( \delta(s, \theta) \)) under the hypotheses of Theorem 5. We may in addition assume that
\[
\delta(s, \theta) < \frac{1}{2} \pi
\] (D.1)

so that the region \( |\varphi| \leq 2\delta(s, \theta) \), and therefore the support of \( \eta \), are subsets of the region \( (-\pi, \pi)^{1 \times m} \).

The bound (C.14) depends only on (2.13) and therefore remains valid; indeed, as remarked in Section 2.5.2, the quantity \( w \) is \( 2\pi \)-periodic in each entry of \( \varphi \), so it is enough to know that \( w \) is continuous. We must establish an analogue of the bound (C.15), which cannot be valid for all \( \varphi \) because of periodicity. From (C.9) and the argument that led to (C.23), we can conclude that, uniformly over suitable neighbourhoods \( U \) and \( W \),
\[
|w(s, \varphi, \theta)| \leq \exp \left( -\frac{1}{2} \delta_0 |\varphi|^2 \right) \quad \text{for} \quad |\varphi| \leq 2\delta(\theta, s). \] (D.2)

On the other hand, by the assumption in Theorem 5,
\[
\max_{\varphi \in (-\pi, \pi)^{1 \times m} : |\varphi| \geq 2\delta(\theta, s)} |w(s, \varphi, \theta)| < 1 \quad \text{for all } (s, \theta) \in \text{int} \mathcal{S}, \] (D.3)
and by continuity and compactness, this maximum is continuous as a function of \((s, \theta)\). It follows that, shrinking \(\delta_0\) if necessary, \(w\) satisfies the bound (C.15) for all \(\varphi \in [-\pi, \pi]^{1 \times m}\).

Let \(\hat{w}(s, \varphi, \theta) = w(s, \varphi, \theta)\mathbb{1}_{[-\pi, \pi]^{1 \times m}}(\varphi)\). Differentiation with respect to \(t\) or \(\tau\) does not affect the indicator, so \(\hat{w}\) satisfies the bounds (C.14)–(C.15). With these bounds given, we can define \(\hat{I}_1, \hat{I}_2, \hat{I}_3\) as in (C.12)–(C.13) with \(w\) replaced by \(\hat{w}\), and the same argument shows that (C.17) holds with \(I_k\) and \(P_n\) replaced by \(\hat{I}_k\) and \(P_{\text{int}, n}\).

The rest of the argument is proceeds as in the proof of Proposition 15: the construction and bounding of \(h\) and \(g\) use only (C.8)–(C.9); the exponentially decaying bound (C.30) still follows from (C.14)–(C.15), applied to \(\hat{w}\) and bounding of \(h\); and the definition and analysis of the functions \(f_1, f_2, f_3\), and of \(q_1, q_2\), are unchanged.

**Proof of Theorem 5 and Proposition 14(e).** Analogues of Corollaries 17 and 22 for \(P_{\text{int}}(\theta, s)\) follow from Proposition 16 by the same argument as in Appendix C. The proofs of Theorem 5 and Proposition 14(e) are then identical to the proofs of Theorems 1–4 and Proposition 14(a)–(d) since all of those proofs use only the result of Corollary 17.

## E Derivatives of \(F\) and proof of Lemma 18

In this section we verify that \(F(s_T^T, \theta_0; y_0, 0) = 0\) and \(\nabla_{s^T, \theta} F(s_T^T, \theta_0; y_0, 0)\) is non-singular, as asserted in the proof of Theorem 2, and we prove Lemma 18.

Since \(\varepsilon = 0\), the assertions \(F_1(s_T^T, \theta_0; y_0, 0) = 0\) and \(F_2(s_T^T, \theta_0; y_0, 0) = 0\) reduce to (2.16) and (2.17), respectively. The gradient of \(F\) with respect to its first two variables (which we combine into a single column vector by concatenating \(s^T\) and \(\theta\)) has the block decomposition

\[
\nabla_{s^T, \theta} F(s_T^T, \theta_0; y_0, 0) = \begin{pmatrix}
\nabla^T F_1(s_T^T, \theta_0; y_0) & \nabla \theta F_1(s_T^T, \theta_0; y_0) \\
\nabla^T F_2(s_T^T, \theta_0; y_0, 0) & \nabla \theta F_2(s_T^T, \theta_0; y_0, 0)
\end{pmatrix}
= \begin{pmatrix}

\nabla s \nabla \theta K_0(s_0; \theta_0) & \nabla \theta K_0(s_0; \theta_0)
\end{pmatrix}^T
\]

(E.1)

with the diagonal blocks symmetric. Abbreviate this as

\[
\nabla_{s^T, \theta} F(s_T^T, \theta_0; y_0, 0) = \begin{pmatrix} A & B \\ B^T & D \end{pmatrix}.
\]

(E.2)

Then, with \(I\) and \(0\) denoting the identity matrix and zero matrix of the indicated sizes,

\[
\begin{pmatrix} I_{m \times m} & 0_{m \times p} \\ -B^TA^{-1} & I_{p \times p} \end{pmatrix} \begin{pmatrix} A & B \\ B^T & D \end{pmatrix} \begin{pmatrix} I_{m \times m} & -B^TA^{-1} \\ 0_{p \times m} & I_{p \times p} \end{pmatrix} = \begin{pmatrix} A & 0_{m \times p} \\ B^T & D - B^TA^{-1}B \end{pmatrix}.
\]

(E.3)

The matrix \(A = K''_0(s_0; \theta_0)\) is positive definite, and we recognise \(D - B^T A^{-1}B\) as the negative definite matrix \(H\) from (2.18). In particular, both are non-singular, and hence \(\nabla_{s^T, \theta} F(s_T^T, \theta_0; y_0, 0)\) is non-singular also, as claimed.

**Proof of Lemma 18.** Consider a solution \(s = s_1, \theta = \theta_1\) of \(F(s_T^T, \theta; y, 1/n) = 0\). The condition \(F_1(s_T^T, \theta; y) = 0\) reduces to the saddlepoint equation (SE\text{SAR}) so that \(s_1 = \hat{s}_0(\theta; y)\). Note that

\[
R'_{x,n}(\theta)^T = F_2(\hat{s}_0^T(\theta; y), \theta; y, 1/n)
\]

(E.4)

so the condition \(F_2(s_T^T, \theta; y, 1/n) = 0\) shows that \(\theta_1\) is a critical point of \(R_{x,n}\).
To complete the proof it suffices to show that, possibly after shrinking $U,V$ and increasing $n_0$, the Hessian $R''_{x,n}(\theta)$ is negative definite for all $\theta \in U,y \in V,n \geq n_0$. From (E.4) and (4.4) we have

$$R''_{x,n}(\theta) = \nabla_\theta \left( F_2(\hat{s}_0^T(\theta; y), \theta; y, 1/n) \right)$$

$$= \nabla_\theta F_2(s_0^T(\theta; y), \theta; y, 1/n)$$

$$- \nabla_\theta^T F_2(s_0^T(\theta; y), \theta; y, 1/n) K_0''(\hat{s}_0(\theta; y); \theta)^{-1} \nabla_\theta K_0(\hat{s}_0(\theta; y); \theta). \quad \text{(E.5)}$$

We note that

$$h(s, \theta, y, \varepsilon) = \nabla_\theta F_2(s^T, \theta; y, \varepsilon) - \nabla_\theta^T F_2(s^T, \theta; y, \varepsilon) K_0''(s; \theta)^{-1} \nabla_\theta K_0(s; \theta) \quad \text{(E.6)}$$

is a continuous function. Moreover $h(s_0, \theta_0, y_0, 0)$ reduces to the negative definite matrix $D - B^T A^{-1} B = H$ from (2.18) and (E.3). By continuity, it follows that $h(s, \theta, y, \varepsilon)$ has only negative eigenvalues for $s, \theta, y, \varepsilon$ in a suitable neighbourhood of $s_0, \theta_0, y_0, 0$. From (E.5) we have $R''_{x,n}(\theta) = h(\hat{s}_0(\theta; y), \theta, y, 1/n)$ which is therefore negative definite for all $\theta, y$ in suitable neighbourhoods and all $n$ large enough, as required.

\[\square\]

## F Proof of Theorem 3

Theorem 3 contains two separate assertions, about $\pi_{\Theta|U,x}$ and about $\hat{\pi}_{\Theta|U,x}$. We prove a stronger statement that removes the restriction $y = y_0$ and also applies to $\hat{\pi}_{\Theta|U,x}$ from Proposition 14(c). To state it, define

$$\hat{\theta}^*_{\text{MLE in } U; 0}(y) = \arg\max_{\theta \in U} \hat{L}_0^*(\theta; y) \quad \text{(F.1)}$$

and note that

$$\hat{\theta}^*_{\text{MLE in } U}(x, n) = \hat{\theta}^*_{\text{MLE in } U; 0}(y)$$

depends only on $y$ and not $n$; see (4.2).

**Proposition 23.** Suppose $(s_0, \theta_0) \in \text{int} \mathcal{S}$ and $y_0 \in \mathcal{Y}_{\theta_0}$ are related as in (2.16), and suppose that (SAR), (2.7), (2.12)–(2.13) and (2.17)–(2.18) hold. Suppose in addition that the prior distribution $\pi_\Theta$ has a probability density function that is continuous and positive at $\theta_0$. Then there exist neighbourhoods $U \subset R$ of $\theta_0$ and $V \subset \mathbb{R}^{m \times 1}$ of $y_0$ such that, for all $y \in V$,

under $\pi_{\Theta|U,x}$, $\hat{\pi}_{\Theta|U,x}$ or $\hat{\pi}^*_{\Theta|U,x}$,

$$\left( \sqrt{n} \left( \Theta - \hat{\theta}_{\text{MLE in } U}(x, n) \right), \sqrt{n} \left( \Theta - \hat{\theta}_{\text{MLE in } U}(x, n) \right), \sqrt{n} \left( \Theta - \hat{\theta}^*_{\text{MLE in } U}(x, n) \right) \right) \quad \text{d} \rightarrow (Z, Z, Z) \quad \text{as } n \rightarrow \infty, \quad \text{(F.3)}$$

where

$$Z \sim \mathcal{N}(0, -H(y)), \quad H(y) = \nabla_\theta^T \nabla_\theta \log \hat{L}_0^*(\hat{\theta}^*_{\text{MLE in } U; 0}(y); y). \quad \text{(F.4)}$$

Note that $H(y)$ generalizes the Hessian $H$ from (2.18), which corresponds to $H(y_0)$.

**Proof.** Start with $U$ and $V$ satisfying the conclusions of Theorem 2 and Proposition 14(b).

Let $f_\Theta(\theta)$ denote the prior density for $\Theta$. Since $f_\Theta(\theta_0) > 0$ and $f_\Theta$ is continuous, we can shrink $U$ if necessary so that $\log f_\Theta(\theta)$ is bounded and continuous over $\theta \in U$. 

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Choose $\hat{\pi}_n$ to be one of the posteriors $\pi_\Theta|_{U^n}$, $\hat{\pi}_\Theta|_{U^n}$ or $\hat{\pi}_\Theta^*|_{U^n}$, let $\hat{L}_n(\theta; x)$ be the corresponding choice out of $L_n(\theta; x)$, $\hat{L}_n(\theta; x)$ or $\hat{L}_n^*(\theta; x)$, respectively, and let $\hat{\theta}(x, n)$ denote the corresponding choice out of $\hat{\theta}_{\text{MLE in }U^n}(x, n)$, $\hat{\theta}_{\text{MLE in }U^n}(x, n)$ or $\hat{\theta}_{\text{MLE in }U^n}(x, n)$, respectively. Let $Q_n(\theta; y)$ be the corresponding choice out of the functions $P_n(\theta, \hat{s}_0(\theta; y))$, $P_n(\theta, \hat{s}_0(\theta; y))$ or the constant function 1, respectively, so that

$$\log \hat{L}_n(\theta; x) = n \log \hat{L}_n^*(\theta; y) + \log Q_n(\theta; y).$$  (F.5)

Note from Theorem 2, Proposition 14(b) and (F.2) that

$$\lim_{n \to \infty} \hat{\theta}(x, n) = \hat{\theta}_{\text{MLE in }U^n}(y)$$  (F.6)

for fixed $y \in V$ and all three choices for $\hat{\theta}$.

The Hessian matrix $H(y_0) = \nabla^T \nabla \log \hat{L}_n(\theta; y_0)$ is negative definite by (2.18), so continuity allows us to shrink $U$ if necessary and choose $\delta > 0$ small enough to ensure that

$$v^T \nabla^T \nabla \log \hat{L}_n^*(\theta; y)v \leq -\delta |v|^2$$  (F.7)

for all $\theta \in U, y \in V$ and $v \in \mathbb{R}^{p \times 1}$.

Shrinking $U$ and $V$ further if necessary, we may assume that $U$ is a bounded convex neighbourhood and that the Hessians $\nabla^2_x \nabla \log Q_n$ and $\nabla^2_y \nabla \log \hat{L}_n^*$ are bounded and uniformly continuous over $\theta \in U$ and $n$ sufficiently large. This is evident if $Q_n(\theta; y)$ is the constant 1 or the function $\hat{P}_n(\theta, \hat{s}_0(\theta; y))$ since both have gradients that do not depend on $n$ and are continuously differentiable functions of $\theta$. For $P_n(\theta, \hat{s}_0(\theta; y))$ the statement follows from Corollary 17.

Let $\hat{f}_{Z_n}(z)$ denote the posterior density function for $Z_n = \sqrt{n}(\Theta - \hat{\theta}(x, n))$ under $\hat{\pi}_n$. By construction, $\hat{f}_{Z_n}$ is chosen to have the form

$$c_n \hat{L}_n(\hat{\theta}(x, n) + z/\sqrt{n}; x) f(\hat{\theta}(x, n) + z/\sqrt{n}) 1_{\{z \in \text{supp} Z_n\}},$$  (F.8)

provided it is possible to choose $c_n = c_n(y, n)$ to make $\int \hat{f}_{Z_n}(z) dz = 1$.

Apply Lagrange’s form of the Taylor series remainder term,

$$g(1) = g(0) + g'(0) + \int_0^1 (1 - u)g''(u)du,$$  (F.9)

with $g(u) = \log \hat{L}_n(\hat{\theta}(x, n) + uz/\sqrt{n}; x)$. By construction, $\hat{\theta}(x, n)$ is a critical point of $\theta \mapsto \hat{L}_n(\theta; x)$, so that $g'(0) = 0$, while

$$g''(u) = n^{-1} z^T \nabla^T \nabla \log \hat{L}_n \left( \hat{\theta}(x, n) + \frac{z}{\sqrt{n}}; x \right) z.$$  (F.10)

Combining (F.5) and (F.9)–(F.10), we compute

$$\log \hat{L}_n \left( \hat{\theta}(x, n) + \frac{z}{\sqrt{n}}; x \right)$$

$$= \log \hat{L}_n(\hat{\theta}(x, n); x) + \int_0^1 (1 - u)z^T \nabla^T \nabla \log \hat{L}_n^* \left( \hat{\theta}(x, n) + \frac{uz}{\sqrt{n}}; y \right) z \, du$$

$$+ \frac{1}{n} \int_0^1 (1 - u)z^T \nabla^T \nabla \log Q_n \left( \hat{\theta}(x, n) + \frac{uz}{\sqrt{n}}; y \right) z \, du.$$  (F.11)
In the right-hand side of (F.11), the first term is constant with respect to \( z \) and does not affect \( \tilde{f}_{Z_n} \). By (F.6) and uniform continuity, the second and third term converge to \( \frac{1}{2}z^TH(y)z \) and 0, respectively. Since \( \tilde{\theta}(x, n) \) converges to an interior point of \( U \), it follows that \( \mathbb{1}_{\{z \in \supp Z_n\}} \) and \( f_\Theta(\tilde{\theta}(x, n) + z/\sqrt{n}) \) converge pointwise to 1 and \( f(\hat{\theta}_{\text{MLE in } U; 0}(y)) \), respectively. Thus
\[
\tilde{L}_n(\tilde{\theta}(x, n) + z/\sqrt{n}; x) f_\Theta(\tilde{\theta}(x, n) + z/\sqrt{n}) \mathbb{1}_{\{z \in \supp Z_n\}} / \tilde{L}_n(\tilde{\theta}(x, n); x)
\]
(F.12)
converges pointwise to \( c(y) \exp \left( \frac{1}{2}z^TH(y)z \right) \), while the bound (F.7) and the boundedness of \( f_\Theta \) and \( \nabla_\theta \nabla_\theta \log Q_n \) show that it is bounded by \( C \exp \left( \left( -\frac{1}{2} \delta + C/n \right) |z|^2 \right) \). By the Dominated Convergence Theorem, it follows that \( \tilde{f}_{Z_n}(z) \) converges to the limiting density \( c' \exp \left( \frac{1}{2}z^TH(y)z \right) \) and \( Z_n \) converges under \( \tilde{\pi}_n \) to the corresponding distribution, which is \( \mathcal{N}(0, -H^{-1}) \) as claimed.

Finally the joint convergence follows because, by Theorem 2 and Proposition 14(b), the differences between the three MLEs are \( O(1/n) \) or \( O(1/n^2) \) and are negligible compared to the \( \sqrt{n} \) scaling.

\[\square\]

**Proof of Theorem 3 and Proposition 14(c).** These are the special case \( y = y_0 \) from Proposition 23, and we note that taking \( y = y_0 \) gives \( \hat{\theta}_{\text{MLE in } U}(x, n) = \hat{\theta}_{\text{MLE in } U; 0}(y_0) = \theta_0 \), so that \( \nabla_\theta \nabla_\theta \log \tilde{L}_0(\hat{\theta}_{\text{MLE in } U; 0}(y_0); y_0) \) reduces to the matrix \( H \) from (2.18).

\[\square\]

**G Proof of Theorem 4**

Theorem 4 follows by an application of the delta method to the function \( G \) from Section 4.3. Note that in the setup of Theorem 4, \( x \) and \( y \) from (SAR) are replaced by \( \xi_n \) and \( \frac{1}{n}\xi_n \) respectively. Write
\[
\tilde{\zeta}_n = \frac{1}{n} \xi_n
\]
(G.1)
so that (2.24) is the assertion
\[
\sqrt{n}(\zeta_n - y_0) \xrightarrow{d} \mathcal{N}(0, \Sigma).
\]
(G.2)

**Proof of Theorem 4 and Proposition 14(d).** The assumptions give a neighbourhood \( V \) of \( y_0 \) and \( n_0 \in \mathbb{N} \) such that \( \hat{\theta}_{\text{MLE in } U}(x, n) \) and \( \hat{\theta}_{\text{MLE in } U}(x, n) \) exist for all \( y \in V \) and \( n \geq n_0 \). Shrinking \( U \), \( V \) and increasing \( n_0 \) if necessary, we can assume that the constructions involving \( G \) from the proof of Theorem 2 in Section 4.3, including Lemma 18, apply for \( y \in V, n \geq n_0 \). (Shrinking \( U \) will not affect the values \( \hat{\theta}_{\text{MLE in } U}(x, n) \) or \( \hat{\theta}_{\text{MLE in } U}(x, n) \) provided they still lie within \( U \).) For \( n \geq n_0 \), define the event
\[
E_n = \{ \zeta_n \in V \} = \left\{ \frac{1}{n} \xi_n \in V \right\}.
\]
(G.3)
The assumption (G.2) implies that \( \zeta_n \) converges in probability to \( y_0 \), so \( \mathbb{P}(E_n) \to 1 \) as \( n \to \infty \). On the event \( E_n \), Lemma 18 gives
\[
\left( s^T(\hat{\theta}_{\text{MLE in } U}(\xi_n, n), \hat{\theta}_{\text{MLE in } U}(\xi_n, n)) \right) = G(\tilde{\zeta}_n, 1/n).
\]
(G.4)
Since $G$ is continuously differentiable,

$$\sqrt{n} \left( \hat{s}^T \left( \theta_{\text{MLE in } U} (\xi_n, n), \xi_n \right) - s_0^T \right)$$

$$= \sqrt{n} \left( G(\hat{\xi}_n, 1/n) - G(y_0, 0) \right)$$

$$= \sqrt{n} \left( \nabla_{y, \varepsilon} G(y_0, 0) \left( \frac{\hat{\xi}_n - y_0}{1/n} \right) + o_P \left( |\hat{\xi}_n - y_0| + 1/n \right) \right)$$

$$= \nabla_y G(y_0, 0) \left[ \sqrt{n} \left( \hat{\xi}_n - y_0 \right) \right] + O(1/\sqrt{n}) + o_P(1) \quad (G.5)$$

where $o_P(B_n)$ denotes a random variable $A_n$ such that $A_n/B_n$ converges to 0 in probability as $n \to \infty$. Restricting our attention to the second sub-block of this vector,

$$\sqrt{n} \left( \theta_{\text{MLE in } U} (\xi_n, n) - \theta_0 \right) = (0_{p \times m} \ I_{p \times p}) \ \nabla_y G(y_0, 0) \left[ \sqrt{n} \left( \hat{\xi}_n - y_0 \right) \right] + o_P(1). \quad (G.6)$$

In particular, $\sqrt{n} \left( \theta_{\text{MLE in } U} (\xi_n, n) - \theta_0 \right)$ will converge to a limiting distribution $Z$ that is asymptotically normal with mean 0.

To calculate the covariance matrix of $Z$, and note that

$$\nabla_y G(y_0, 0) = \nabla_{y, \varepsilon} G(y_0, 0) \left( I_{m \times m} \right)_{01 \times m}$$

$$= \left[ - \left( \nabla_{sT, \theta} F(s_0^T, \theta_0; y_0, 0) \right)^{-1} \nabla_{y, \varepsilon} F(s_0^T, \theta_0; y_0, 0) \right] \left( I_{m \times m} \right)_{01 \times m} \quad (G.7)$$

We compute

$$\nabla_{y, \varepsilon} F(s_0^T, \theta_0; y_0, 0) \left( I_{m \times m} \right)_{01 \times m} = - \left( I_{m \times m} \right)_{0p \times m} \quad (G.8)$$

and recalling (E.2)–(E.3) in which $D - B^T A^{-1} B = H$,

$$\left( 0 \ I \right) \ \nabla_G(y_0, 0) = - \left( 0 \ I \right) \left( \nabla_{sT, \theta} F \right)^{-1} \left[ \left( \nabla_{y, \varepsilon} F \right) \left( I \right) \right]$$

$$= - \left( 0 \ I \right) \left[ \left( I \ - A^{-1} B \right) \left( A^{-1} \ 0 \right) \left( 0 \ I \right) \ - \left( 0 \ I \right) \right]$$

$$= \left( 0 \ I \right) \left( A^{-1} \ 0 \right) \left( 0 \ I \right) \left( 0 \ I \right) = -H^{-1} B^T A^{-1}. \quad (G.9)$$

From (G.2), it follows that the covariance matrix of $Z$ is $H^{-1} B^T A^{-1} \Sigma \left( H^{-1} B^T A^{-1} \right)^T$. Since $H$ and $A$ are symmetric, this reduces to the expression in part (a).

To handle the joint convergence in Theorem 4(a) and Proposition 14(d), we again observe that the differences between the three MLEs are negligible in the $\sqrt{n}$ scaling of Theorem 4.

Finally part (b) follows from the observation, discussed in Section 2.5.4, that $s_0 = 0$ gives $D = 0$ and $H = -B^T A^{-1}$. If in addition $\Sigma = A$ then $H^{-1} B^T A^{-1} \Sigma A^{-1} B H^{-1}$ simplifies to $-H^{-1}$, as claimed. \hfill $\square$

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