On the error in Laplace approximations of high-dimensional integrals

Helen Ogden
University of Southampton, UK

Summary
Laplace approximations are commonly used to approximate high-dimensional integrals in statistical applications, but the quality of such approximations as the dimension of the integral grows is not well understood. In this paper, we prove a new result on the size of the error in first- and higher-order Laplace approximations, and apply this result to investigate the quality of Laplace approximations to the likelihood in some generalized linear mixed models.

Keywords: Asymptotic approximation; Intractable likelihood; Generalized linear mixed model

1 Introduction
Integrals of the form
\[ L = \int_{\mathbb{R}^d} \exp\{-g(u)\} du \] (1)
are frequently encountered in statistical applications, where \( g(.) \) is a smooth function with a unique minimum. For example, the likelihood function for a generalized linear mixed model is of this form, where \( u \) is a vector of random effects. Integrals of this type are also common in Bayesian applications, for example as marginal likelihoods used for model comparison.

Laplace approximations are often used to approximate integrals of form (1). Suppose that \( g(u) \) grows at rate \( n \). Often \( g(u) \) is a sum with one term for each observation, so \( n \) is the sample size. If \( d \) is fixed as \( n \to \infty \), many results on the quality of the Laplace approximation are available: see [Small (2010)] for a review. However, in many examples of interest, \( d \) and \( n \) tend to infinity simultaneously, and there are very few results available on the quality of Laplace approximations in this setting.

[Shun and McCullagh (1995)] provide a formal expansion for integrals of type (1). By studying the size of various terms in this expansion, they conjecture that the first-order Laplace approximation should be reliable if \( d = o(n^{1/3}) \), under the assumption that all derivatives of \( g(.) \) grow at rate \( n \). This condition is typically not met for generalized linear mixed models, and we give an example in which \( d = o(n^{1/3}) \) but the error in the first-order Laplace approximation grows with \( n \).
In Section 2, assuming alternative conditions on \( g(.) \), we develop a new result on the error in Laplace approximations of various orders to integrals of type (1). Our result is motivated by a two-level random intercept model with \( n_j \) observations on items in the \( j \)th cluster, for which the likelihood factorizes into a product of terms

\[
L = \prod_{j=1}^{d} \int_{-\infty}^{\infty} \exp\{-g_j(u_j)\} du_j,
\]

where each \( g_j(u_j) \) is a sum over \( n_j \) terms. In this case, we could use existing results on the error of Laplace approximations to one-dimensional integrals to show that the error in the first-order Laplace approximation to the integral is \( O(\sum_{j=1}^{d} n_j^{-1}) \). We show that a version of this result also holds more generally, and find similar expressions for the error in higher-order Laplace approximations. In Section 3, we apply these results to study the quality of Laplace approximations of the likelihood for some generalized linear mixed models, including a multilevel random intercept model with any number of levels of hierarchy.

2 Error in the log-integral approximation

2.1 A series expansion for the log-integral

Shum and McCullagh (1995) give a series expansion for the log-integral \( \ell = \log L \). We use their expansion here, expressed with slightly different notation. We write

\[
\ell = \tilde{\ell}_1 + \sum_{l=1}^{\infty} e_l,
\]

where \( \tilde{\ell}_1 \) is the first-order Laplace approximation to the log-integral, and \( e_l \) are contributions to the error in this approximation of size decreasing with \( l \), which we define in Section 2.2.

The first-order Laplace approximation to the log-integral is

\[
\tilde{\ell}_1 = -\frac{1}{2} \log \det(g^{(2)}) + \frac{d}{2} \log(2\pi) - g(\hat{u})
\]

where \( \hat{u} = \arg \min_{u \in \mathbb{R}^d} \{ g(u) \} \) and \( g^{(2)} = g''(\hat{u}) \) is the matrix of second derivatives of \( g(.) \) with respect to \( u \), evaluated at \( \hat{u} \).

Based on the decomposition (2), we may also define an order-\( k \) Laplace approximation to the log-integral, for \( k \geq 2 \), as

\[
\tilde{\ell}_k = \tilde{\ell}_1 + \sum_{l=1}^{k-1} e_l.
\]

What is meant by the order of a Laplace approximation is not standard across the literature: our definition is made by grouping together terms in a series expansion to the log-integral in terms of their asymptotic order. This is a different notion of order than that used by Raudenbush et al. (2000), who group together terms according to the number of derivatives required to compute them.
In this paper, we study the errors in these Laplace approximations to the log-integral
\[
e_k = \hat{\ell}_k - \ell = - \sum_{l=k}^{\infty} e_k.
\]

2.2 An expansion over bipartitions

Shun and McCullagh (1995) give a series expansion for the log-integral in terms of particular bipartitions. For positive integers \(v\) and \(m\), define the set of \(M\)-bipartitions \(M_{v,m}\) to be all \((P, Q)\) such that \(P = (p_1 | \ldots | p_v)\) and \(Q = (q_1 | \ldots | q_m)\) are both partitions of \(\{1, \ldots, 2m\}\), such that each block of \(P\) contains at least three elements and each block of \(Q\) contains exactly two elements.

For each \((P, Q) \in M_{v,m}\), define a corresponding graph \(G(P, Q)\) with vertices \(1, \ldots, 2m\), and an edge between each pair of vertices contained in the same block of either \(P\) or \(Q\). If \(G_{P,Q}\) is a connected graph, say that \((P, Q)\) is a connected bipartition, and write \((P, Q) \in M^C_{v,m}\). We define the level of \((P, Q) \in M_{v,m}\) to be \(l = m - v\), and write \(M^C_l\) for all connected level-\(l\) \(M\)-bipartitions.

For a vector of indices \(I\), write \(g_I(u) = \nabla u^I g(u)\) and \(g_I = g_I(\hat{u})\). Let \(g^{(k)}\) be the \(k\)-dimensional array with entries \(g_{j_1, \ldots, j_k} = g_{j_1, \ldots, j_k}\), and write \(g^{jk} = (g^{(2)})^{-1}_{jk}\). Then define
\[
e_{P,Q} = \frac{(-1)^v}{(2m)!} \sum_{j \in [1 : d]^{2m}} g_{jp_1} \ldots g_{jp_v} g^{j_{k_1}} \ldots g^{j_{km}},
\]
where \([1 : d]^{2m} = \{(j_1, \ldots, j_{2m}) : j_l \in \{1, \ldots, d\}\}\), and \(j_p\) is the sub-vector of \(j = (j_1, \ldots, j_{2m})\) corresponding to the indices in \(p\).

We may write the level-l contribution to the log-integral \(e_l\) as a sum of contributions from each connected level-l \(M\)-bipartition, as
\[
e_l = \sum_{(P, Q) \in M^C_l} e_{P,Q}.
\]

2.3 The level-1 contribution

To demonstrate the definitions in Section 2.2, we find the level-1 contribution \(e_1\), used in the second-order Laplace approximation.

There are three types of bipartitions in \(M^C_1\): \((P_1, Q_1)\), where \(P_1 = (1 2 3 4)\) and \(Q_1 = (1 2 | 3 4)\); \((P_2, Q_2)\), where \(P_2 = (1 2 3 | 4 5 6)\) and \(Q_2 = (1 2 3 | 4 5 6)\); and \((P_3, Q_3)\) where \(P_3 = P_2\) and \(Q_3 = (1 4 5 6 | 2 3)\). While there are other bipartitions in \(M^C_1\), they are all similar to one of these three, in that they may be obtained by rearranging the labels \(\{1, \ldots, 2m\}\), and so give the same contribution \(e_{P,Q}\). For example, the bipartition \(P_1^* = (1 2 3 4)\), \(Q_1^* = (1 3 4 2)\) may be obtained from \((P_1, Q_1)\) by exchanging 2 and 3, and \(e_{P_1^*, Q_1^*} = e_{P_1, Q_1}\).
From (3), we have
\[ e_{P_1,Q_1} = -\frac{1}{4!} \sum_{j_1,\ldots,j_4} g_{j_1,j_2,j_3,j_4} g_{j_1,j_2} g_{j_3,j_4} \]
\[ e_{P_2,Q_2} = \frac{1}{6!} \sum_{j_1,\ldots,j_6} g_{j_1,j_2,j_3} g_{j_4,j_5,j_6} g_{j_1,j_2,j_3} g_{j_4,j_5,j_6} \]
\[ e_{P_3,Q_3} = \frac{1}{6!} \sum_{j_1,\ldots,j_6} g_{j_1,j_2,j_3} g_{j_4,j_5,j_6} g_{j_1,j_2,j_3} g_{j_4,j_5,j_6} \]

(5)

McCullagh (1987) lists 4 bipartitions similar to \((P_1,Q_2)\), 9 similar to \((P_2,Q_2)\) and 6 similar to \((P_3,Q_3)\), so the level-1 contribution is \(e_1 = 3e_{P_1,Q_1} + 9e_{P_2,Q_2} + 6e_{P_3,Q_3}\), and the second-order Laplace approximation to the log-likelihood is \(\ell_2 = \ell_1 + e_1\).

There may be more efficient ways to compute \(e_1\) than direct computation of the sums in (5). For example, Zipunnikov and Booth (2011) describe a more efficient method for computing these terms for a generalized linear mixed model.

2.4 Asymptotic order of terms

Write \(a = \Theta(b)\) if \(a = O(b)\) and \(a^{-1} = O(b^{-1})\), so \(a\) grows at the same rate as \(b\). For a random variable \(A\), write \(A = \Theta_p(b_n)\) if \(A = O_p(b_n)\) and \(A^{-1} = O_p(b_n^{-1})\).

We use a particular notion of a random array being order 1 in probability. Suppose \(A\) is a \(k\)-dimensional array, with entries \(A_{j_1,\ldots,j_k}\) for each \(j_i \in \{1, \ldots, d\}\). If \(k = 1\), say \(A = O_p^*(1)\) if \(A_j = O_p(1)\) for each \(j = 1, \ldots, d\). If \(k \geq 2\), let
\[ A_{i}^{(j)} = \sum_{j_1=1}^{d} \ldots \sum_{j_{i-1}=1}^{d} \sum_{j_{i+1}=1}^{d} \ldots \sum_{j_k=1}^{d} |A_{j_1,\ldots,j_{i-1},j_i,j_{i+1},\ldots,j_k}|, \]
and say \(A = O_p^*(1)\) if \(A_i^{(j)} = O_p(1)\) for each \(i = 1, \ldots, k\) and \(j = 1, \ldots, d\).

If \(A\) is a diagonal array, then \(A = O_p^*(1)\) if the diagonal entries \(A_{j,j,\ldots,j} = O_p(1)\).

2.5 Assumptions

We assume that \(g(.)\) in (11) satisfies some conditions.

**Condition 1.** 
\(g(.)\) is a smooth function with a unique minimum.

For a given choice of normalizing terms \(n_1, \ldots, n_d\), and for each vector of indices \(I\), define the normalized derivatives
\[ f_I = g_I \prod_{j \in I} n_j^{-1/|I|}, \]
and write \(f^{(k)}\) for the \(k\)-dimensional array with entries \(f^{(k)}_{j_1,\ldots,j_k} = f_{j_1,\ldots,j_k}\). We write \(f_{jk} = [(f^{(2)})^{-1}]_{jk}\).

**Condition 2.** 
There is some choice of normalizing terms \(n_1, \ldots, n_d\) such that the normalized derivative arrays \(f^{(k)}\) satisfy \(f^{(k)} = O_p^*(1)\) for all \(k \geq 3\), and \([f^{(2)}]^{-1} = O_p^*(1)\).

The normalizing terms are often chosen so that \(g_{jj} = \Theta_p(n_j)\), and we may think of \(n_j\) as an effective sample size for \(u_j\).
2.6 Error in log-integral approximations

We state here our main result, which is proved in Appendix A.

**Theorem 1.** Suppose $L$ is of form (1), where $g(.)$ satisfies Conditions 1 and 2 for some choice of normalizing terms $n_1, \ldots, n_d$. Then the error in the order-$k$ Laplace approximation to $\log L$ is $\epsilon_k = O_p(\sum_{j=1}^{d} n_j^{-k})$.

2.7 Linear reparameterizations

Laplace approximations are invariant to linear reparameterizations. That is, if $v = Au$, where $A$ is an invertible $d \times d$ matrix, then writing $g_v(v) = g(A^{-1}v) + \log \det(A)$, and

$$L^{(v)} = \int_{\mathbb{R}^d} \exp\{-g_v(v)\} dv,$$

we have $L^{(v)} = L$, and the order-$k$ Laplace approximation of $L$ is unchanged by the reparameterization, so that $\tilde{L}_k^{(v)} = \tilde{L}_k$.

In many situations, Condition 2 does not hold in the original parameterization, but does hold after making a suitable linear reparameterization, so we may still apply Theorem 1. We give an example of this in Section 3.5.

3 Application to likelihood approximation for generalized linear mixed models

3.1 The model

In a generalized linear mixed model, the distribution of the response $Y = (Y_1, \ldots, Y_n)$ is determined by a linear predictor $\eta = (\eta_1, \ldots, \eta_n)$. Conditional on $\eta$, the components $Y_i$ of the response are independent, with known density function $f(y_i|\eta_i)$. We assume an exponential family with canonical link, so that

$$\log f(y_i|\eta_i) = y_i \eta_i - b(\eta_i) a_i(\phi),$$

where $b(.)$ is a smooth and convex function, $a_i(\phi) > 0$, and $\phi$ is the dispersion parameter, which we assume here to be known. The linear predictor is modelled as $\eta = X\beta + Zu$, where $X \in \mathbb{R}^{n \times p}$ and $Z \in \mathbb{R}^{n \times d}$ are design matrices, $\beta \in \mathbb{R}^p$ is a vector of fixed effects, and $u \in \mathbb{R}^d$ is a vector of random effects. We assume that $u \sim N_d(0, \Sigma(\psi))$, where $\psi \in \mathbb{R}^q$ is an unknown parameter, and write $\theta = (\beta, \psi)$ for the full vector of unknown parameters.

3.2 The likelihood

The likelihood for this model is

$$L(\theta) = \int_{\mathbb{R}^d} \exp\{-g(u; \theta)\} du,$$

where

$$g(u; \theta) = h(u; \beta) - \log \phi_d(u; 0, \Sigma(\psi)),$$
\[ h(u; \beta) = \sum_{i=1}^{n} - \log f(y_i | \eta_i = X_i^T \beta + Z_i^T u) \]
\[ = \sum_{i=1}^{n} \frac{b(X_i^T \beta + Z_i^T u) - y_i(X_i^T \beta + Z_i^T u)}{a_i(\phi)} \]  

and \( \phi_d(\cdot; \mu, \Sigma) \) is the \( \mathcal{N}_d(\mu, \Sigma) \) density function. The \( d \)-dimensional integral in (9) is typically intractable, except in the special case of a linear mixed model where \( Y_i | \eta_i \) are normally distributed. Because of this intractability, it is common to use some numerical approximation \( \bar{L}(\theta) \) to the likelihood, and first-order Laplace approximation is often used. For example, by default the \texttt{lme4} R package (Bates et al., 2015) uses a first-order Laplace approximation to the likelihood for inference, and the integrated nested Laplace approximations of Rue et al. (2009) is a Bayesian approach based on a Laplace approximation to the likelihood.

### 3.3 Assumption checking

In order to apply Theorem 1 to the likelihood of a generalized linear mixed model, we will first have to show that \( g(\cdot) \) as defined in (7) satisfies Conditions 1 and 2. We drop \( \theta \) from the notation, so that (6) is of form (1).

We can show Condition 1 holds in all cases. The proof is in Appendix B.

**Proposition 1.** Let \( g(u) \) be as defined in (7), where \( \Sigma \) is a positive definite matrix. Then \( g(\cdot) \) satisfies Condition 1.

We need to show that Condition 2 holds on a case-by-case basis. In our examples, we choose the normalizing term \( n_j \) to be the number of observations which involve \( u_j \).

### 3.4 A two-level random intercept model

We consider a two-level random intercept model, which is a special case of the generalized linear mixed model of Section 3.1 in which each observation \( i \) is contained in a cluster \( c(i) \). Observations in the same cluster \( j \) are correlated by a shared random effect \( u_j \). The linear predictor is \( \eta_i = x_i^T \beta + u_{c(i)} (i = 1, \ldots, n) \), where we suppose the \( u_j \) are independent \( \mathcal{N}(0, \sigma^2) \) random variables. In the notation of Section 3.1 we have \( Z_{i,c(i)} = 1, \) and \( Z_{i,j} = 0 \) if \( j \neq c(i) \) and \( \Sigma = \sigma^2 I \), where \( I \) is an identity matrix.

In this special case, the likelihood (6) simplifies into a product of one-dimensional integrals

\[ L(\theta) = \prod_{j=1}^{d} \int \prod_{i:c(i)=j} f(y_i | \eta_i = x_i^T \beta + u_j) \phi(u_j; 0, \sigma^2) du_j. \]

The log-likelihood may be written as a sum

\[ \ell(\theta) = \sum_{j=1}^{d} \log \int \prod_{i:c(i)=j} f(y_i | \eta_i = x_i^T \beta + u_j) \phi(u_j; 0, \sigma^2) du_j, \]

so \( \epsilon_k \) is a sum of separate error terms.
Proposition 2. Suppose we have a two-level random intercept model, with \( n_j \) observations on cluster \( j \), for \( j = 1, \ldots, d \). The error in the order-\( k \) Laplace approximation to the log-likelihood is
\[
\varepsilon_k(\theta) = \tilde{\ell}_k(\theta) - \ell(\theta) = O_p\left( \sum_{j=1}^{d} n_j^{-k} \right).
\]

Proof. The derivative arrays \( g^{(k)} \) are diagonal for all \( k \), with diagonal entries \( g_{jj}\ldots j = \Theta(n_j) \), so Condition 2 holds with normalizing terms \( n_1, \ldots, n_d \). Theorem 1 gives that \( \varepsilon_k(\theta) = O_p\left( \sum_{d} n_j^{-k} \right) \), as required.

In the balanced case, where all \( n_j = nd^{-1} \), \( \varepsilon_k = O_p(d^{k+1}n^{-k}) \). This tends to zero as \( n \to \infty \) if \( d = o(n^{(k+1)/k}) \). The error in the first-order Laplace approximation tends to zero if \( d = o(n^{1/2}) \).

In an unbalanced case, the result can be quite different. As an extreme example, suppose \( n_j = \begin{cases} \log d & \text{if } j = 1, \ldots, d-1 \\ n - (d-1) \log d & \text{if } j = d, \end{cases} \)

where \( n > d \log d \). Then
\[
\varepsilon_1 = O_p((d-1)(\log d)^{-1} + (n - (d-1) \log d)^{-1}) = O_p(d(\log d)^{-1}),
\]
which tends to infinity as \( d \to \infty \), now matter how large \( n \) is relative to \( d \). For example, if \( n = d^4 \), then \( d = o(n^{1/3}) \), but \( \varepsilon_1 \to \infty \).

3.5 A multilevel random intercept model

Suppose that each observation \( i \) is contained in a level-2 cluster \( c_2(i) \), and that each level-2 cluster \( j \) is itself contained within a hierarchy of higher-level clusters, \( c_l(j) \), \( j = 3, \ldots, L \). The clusters are nested within one another, so that if \( c_l(j) = c_l(k) \), then \( c_{l+1}(j) = c_{l+1}(k) \). The linear predictor is
\[
\eta_i = x_i^T \beta + u_{c_2(i)}^{(2)} + \sum_{l=3}^{L} u_{c_l(c_2(i))}^{(l)} (i = 1, \ldots, n),
\]
where we assume \( u_j^{(l)} \sim N(0, \sigma_l^2) \), \( l = 2, \ldots, L \), with all the \( u_j \) independent. Suppose that there are \( d \) level-2 clusters in total, and \( d_l \) level-\( l \)-clusters, for each \( l = 3, \ldots, L \). It is no longer possible to write the log-likelihood as a sum of one-dimension log-integrals as in [8]. Since an accurate approximation to the exact log-likelihood is no longer readily available, it is important to understand the quality of the Laplace approximation in this case.

Condition 2 does not hold for this parameterization, so we define a new parameterization of the model. Let \( v_j = u_j^{(2)} + \sum_{l=3}^{L} u_j^{(l)} \) for \( j = 1, \ldots, d \). We have \( \eta_i = x_i^T \beta + v_{c_2(i)} \), where there are now a total of \( d \) random effects, rather than \( d + d_3 + \ldots + d_L \) in the original parameterization. We have reduced the
structure to the two-level random intercept model of Section 3.4, except now $v \sim N_d(0, \Sigma)$, where

$$
\Sigma_{jk} = \begin{cases} 
\sigma_2^2 + \sigma_3^2 + \ldots + \sigma_L^2 & \text{if } j = k \\
\sigma_3^2 + \ldots + \sigma_L^2 & \text{if } j \neq k, \text{ but } c_3(j) = c_3(k) \\
\vdots & \vdots \\
\sigma_L^2 & \text{if } c_{L-1}(j) \neq c_{L-1}(k), \text{ but } c_L(j) = c_L(k) \\
0 & \text{if } c_L(j) \neq c_L(k). 
\end{cases}
$$

Proposition 3. Suppose we have an $L$-level random intercept model with independent random effects, with $n_j$ observations in level-2 cluster $j$, for $j = 1, \ldots, d$. The error in the order-$k$ Laplace approximation to the log-likelihood is

$$
\epsilon_k(\theta) = \hat{\ell}_k(\theta) - \ell(\theta) = O_p \left( \sum_{j=1}^d n_j^{-k} \right).
$$

The proof is in Appendix B.

The asymptotic order of the error in a Laplace approximation to the log-likelihood depends on the number of observations in each of the level-2 clusters, but not on how these level-2 clusters are grouped into higher-level clusters.

3.6 Impact on approximate likelihood inference

When an approximate likelihood $\hat{L}(\theta)$ is used for inference, the impact of the error in the likelihood approximation on the resulting inference is of more interest than the size of that error itself. If the error in the log-likelihood $\epsilon(\theta) = \log \hat{L}(\theta) - \log L(\theta)$ tends to zero in probability, uniformly in $\theta$, [Douc et al. (2004)] show that the approximate likelihood estimator $\hat{\theta}$ will be fully efficient, and have the same first-order asymptotic distribution as the maximum likelihood estimator. In our examples, if

$$
\sum_{j=1}^d n_j^{-k} \to 0 \text{ as } d \to \infty
$$

we expect the order-$k$ Laplace estimator to be fully efficient. In order to make the argument rigorous, we would need to show that the supremum of the error in log-likelihood in some region around the true parameter value tends to zero.

However, condition (10) is likely to be stronger than necessary for a order-$k$ Laplace estimator to be fully efficient. [Ogden (2017)] gives conditions on the size of the error in the score function $\nabla_{\theta} \epsilon(\theta)$ which ensure that inference with an approximate likelihood retains the same first-order properties as inference with the exact likelihood. By studying this error in score, it should be possible to show that the order-$k$ Laplace estimator is fully efficient under a weaker condition than (10). Some modification of the results of [Ogden (2017)] would be required before they could be used in this case, as information on different components of the parameter vector may grow at different rates [Nie (2007)].
Appendix A  Proof of main result

To prove Theorem 1 we aim to find the size of the contribution from each bipartition \((P, Q)\).

**Lemma 1.** Suppose Condition 2 holds. For each fixed bipartition \((P, Q) \in \mathcal{M}_d^C\)
\[ e_{P, Q} = O_p\left(\sum_{j=1}^d n_j^{-l}\right). \]

Given Lemma 1, the proof of Theorem 1 is straightforward:

**Proof of Theorem 1.** By Lemma 1 we have \(e_{P, Q} = O_p\left(\sum_{j=1}^d n_j^{-l}\right)\) for each fixed bipartition \((P, Q) \in \mathcal{M}_d^C\). Combining the contributions from each bipartition in \(\mathcal{M}_d^C\), we have \(e_l = O_p\left(\sum_{j=1}^d n_j^{-l}\right)\), so \(e_k = -\sum_{l=k}^\infty e_k = O_p\left(\sum_{j=1}^d n_j^{-l}\right)\), as required. \(\square\)

In order to prove Lemma 1 we need some auxiliary results.

**Proposition 4.** Let \((P, Q)\) be a fixed \((v, 2m)\) bipartition. For each \(j = (j_1, \ldots, j_{2m}) \in [1:d]^{2m}\), write \(A_{P, Q}(j) = f_{j_{p,1}} \cdots f_{j_{p,n}} f_{j_{q,1}} \cdots f_{j_{q,n}}\). Then
\[ e_{P, Q} = \frac{(-1)^v}{(2m)!} \sum_{j \in [1:d]^{2m}} n_{j_{1}}^{c_1} \cdots n_{j_{2m}}^{c_{2m}} A_{P, Q}(j) \]
where \(\sum_{j=1}^{2m} c_j = -l\), and each \(c_j < 0\).

**Proof.** We may write
\[ e_{P, Q} = \frac{(-1)^v}{(2m)!} \sum_{j \in [1:d]^{2m}} \prod_{p \in P} \prod_{k \in f_p} n_k^{1/|p|} f_{j_{p,1}} \cdots f_{j_{p,n}} \prod_{q \in Q} \prod_{l \in f_q} n_l^{-1/2} f_{j_{q,1}} \cdots f_{j_{q,n}} \]
for some \(c_1, \ldots, c_{2m}\). We have \(c_i = -\frac{1}{2} + \frac{1}{|p|}\), for whichever \(p\) contains \(i\), so \(c_i < 0\) as \(|p| \geq 3\). We have
\[ \sum_{i=1}^{2m} c_i = -m + \sum_{p \in P} \sum_{i \in p} \frac{1}{|p|} = -m + \sum_{p \in P} 1 = -m + v = -l \]
which gives the result. \(\square\)

**Proposition 5.** Suppose \(A = O_p^*(1)\) and \(B = O_p^*(1)\), and \(C\) is the \(k\)-dimensional array with entries \(C_{j} = A_{j_1} B_{j_2}\), where \(j = (j_1, \ldots, j_k)\), and \(S, T \subseteq \{1, \ldots, k\}\), such that \(S \cup T = \{1, \ldots, k\}\). If \(S \cap T \neq \emptyset\), then \(C = O_p^*(1)\).

**Proof.** We proceed by induction on \(k = \dim(C) = |S \cup T|\).

In the case \(k = 1\), we have \(S = T\), since \(S \cap T \neq \emptyset\). So \(C_{j_1} = A_{j_1} B_{j_1} = O_p(1)\), so \(C = O_p^*(1)\).

Now we suppose the hypothesis is true for \(\dim(C) = k - 1\), and consider \(\dim(C) = k \geq 2\).
We have
\[ C_{ji}^a = \sum_{j_i \neq i} |C_{ji}| = \sum_{j_i \neq i, a} \sum_j |C_{ji}|. \]
Writing \( j-a = (j_1, \ldots, j_{a-1}, j_{a+1}, \ldots, j_k) \) and \( C_{j-a}^{-a} = \sum_{j_a} |C_j| \), if we can show that \( C^{-a} = O_p^*(1) \) for some \( a \neq i \), then
\[ C_{ji}^a = \sum_{j_i \neq i, a} C_{j-a}^{-a} = O_p(1), \]
so that \( C = O_p^*(1) \).

\( C^{-a} \) has entries
\[ C_{j-a}^{-a} = \sum_{j_a} |A_{j,a} B_{j,a}| = \begin{cases} |B_{j,a}^T| \sum_{j_a} |A_{j,a}| & \text{if } a \in S, a \notin T \\ |A_{j,a}^T| \sum_{j_a} |B_{j,a}| & \text{if } a \notin S, a \in T \\ \sum_{j_a} |A_{j,a}^T B_{j,a}^T| & \text{if } a \in S, a \in T \end{cases} \]
In the first case, we must have \( \dim(A) \geq 2 \), otherwise \( S = \{a\} \) and \( S \cap T = \emptyset \), which would be a contradiction. Since \( A = O_p^*(1) \), the array \( A^{-a} \) with entries \( A_{j,a}^{-a} = \sum_{j_a} |A_{j,a}| \) must also be \( O_p^*(1) \). So the array \( C^{-a} \) with entries \( C_{j-a}^{-a} = |B_{j,a}^T| A_{j,a}^{-a} \) is \( O_p^*(1) \), by the induction hypothesis, since \( \dim(C^{-a}) = k-1 \).
Similarly, in the second case \( C^{-a} = O_p^*(1) \). In the third case,
\[ C_{j-a}^{-a} = \sum_{j_a} |A_{j,a} B_{j,a}| \leq \sum_{j_a} |A_{j,a}| \sum_{j_a} |B_{j,a}| = A_{j,a}^{-a} B_{j,a}^{-a} \]
by the Cauchy–Schwarz inequality. So \( C^{-a} = O_p^*(1) \), by the induction hypothesis.

In all cases \( C^{-a} = O_p^*(1) \), so \( C = O_p^*(1) \), as required. \( \square \)

**Proposition 6.** Suppose Condition 3 holds. Let \( (P, Q) \) be a fixed \((v, 2m)\) bipartition. Then \( A_{P,Q} = O_p^*(1) \).

**Proof.** We have \( A_{P,Q}(j) = \prod_{p \in P} f_{j_p} \prod_{q \in Q} f_{j_q} \). Since \( f^{(k)} = O_p^*(1) \) for \( k \geq 3 \) and \( \lfloor f^{(2)} \rfloor^{-1} = O_p^*(1) \), \( A_{P,Q} \) is a product of \( O_p^*(1) \) arrays.

We build up this product one term at a time, at each step applying Proposition 5 to show that the product remains \( O_p^*(1) \).

We start with an arbitrary \( p_1 \in P \), and choose \( q_1 \in Q \) such that one element of \( q_1 \) is in \( p_1 \), and the other is not in \( p_1 \), and therefore must be in some other block \( p_2 \in P \). If \( v > 1 \), it will always be possible to find such a \( q \), because \((P, Q)\) is a connected bipartition, so blocks of \( P \) (which form disjoint clusters in \( G_{P,Q} \)) are connected by blocks of \( Q \).

Let \( S^1 \) be the array with entries \( S_{j_1 q_1}^1 = f_{j_1} f_{j_1 q_1} \). Then \( S^1 = O_p^*(1) \) by Proposition 5 as \( p_1 \cap q_1 \neq \emptyset \). Let \( T^1 \) be the array with entries \( T_{j_2 q_1}^1 = f_{j_2} S_{j_2 q_1}^1 \). Then \( T^1 = O_p^*(1) \), as \( p_2 \cap (p_1 \cup q_1) = p_2 \cap q_1 \neq \emptyset \).

We continue to choose alternating terms from blocks of \( Q \) and \( P \), at step \( k \) choosing a block \( q_k \) with one entry in \( p_1 \cup \ldots \cup p_k \), and the other entry in a new block \( p_{k+1} \). At each stage \( k \) we have \( S_{j_{k-1} q_1}^k = f_{j_{k-1}} T_{j_{k-1} q_1}^{k-1} \) and \( T_{j_k q_{k+1}}^k = f_{j_k} S_{j_k q_{k+1}}^k \), where \( S^k = O_p^*(1) \) and \( T^k = O_p^*(1) \).
We continue until we have included all blocks of \( P \), and have \( T^{v-1}_{j_{p_1},\ldots,j_{p_v}} = T^v_{j} \) and \( T^v = O^*_p(1) \). We have already included terms from \( v-1 \) blocks of \( Q \). We may multiply in the remaining \( 2m - v + 1 \) blocks of \( Q \) while retaining an \( O^*_p(1) \) array by Proposition 5 as \( T^v = \) an array on all indices \( j_1,\ldots,j_{2m} \), and \( q \cap (1:2m) = q \neq \emptyset \) for each \( q \in Q \). So \( A_{P,Q} = O^*_p(1) \), as required. \( \blacksquare \)

**Proof of Lemma 4** By Proposition 4

\[
|e_{P,Q}| = \frac{1}{(2m)!} \left| \sum_{j \in [1:d]^{2m}} n_{j_1}^{c_1} \cdots n_{j_{2m}}^{c_{2m}} A_{P,Q}(j) \right|
\]

\[
\leq \frac{1}{(2m)!} \sum_{j \in [1:d]^{2m}} n_{j_1}^{c_1} \cdots n_{j_{2m}}^{c_{2m}} |A_{P,Q}(j)|.
\]  

(11)

We apply the weighted form of the inequality of arithmetic and geometric means, which states that given non-negative numbers \( x_1,\ldots,x_n \) and non-negative weights \( w_1,\ldots,w_n \) with \( \sum_i w_i = 1 \),

\[
\prod_{i=1}^n x_i^{w_i} \leq \sum_{i=1}^n w_i x_i.
\]

Here, we let \( n = 2m \), \( x_i = n_{j_i}^{-l} \) and \( w_i = -c_i/l \), to give that

\[
n_{j_1}^{c_1} \cdots n_{j_{2m}}^{c_{2m}} \leq \sum_{i=1}^{2m} w_i n_{j_i}^{-l}.
\]  

(12)

Putting (12) back into (11) gives

\[
|e_{P,Q}| \leq \frac{1}{(2m)!} \sum_{j \in [1:d]^{2m}} \sum_{i=1}^{2m} w_i n_{j_i}^{-l} |A_{P,Q}(j)|
\]

\[
= \frac{1}{(2m)!} \sum_{i=1}^{2m} \sum_{j_1}^d w_i n_{j_1}^{-l} \sum_{j_i+1}^{j_{2m}} |A_{P,Q}(j)|
\]

\[
= \frac{1}{(2m)!} \sum_{i=1}^{2m} \sum_{j_1}^d w_i n_{j_1}^{-l} A_{j_i}
\]

\[
= \frac{1}{(2m)!} \sum_{i=1}^{2m} O_p \left( \sum_{j_1}^d n_{j_i}^{-l} \right) = O_p \left( \sum_{j_1}^d n_{j_i}^{-l} \right)
\]

since \( m \) is fixed as \( d \to \infty \). \( \blacksquare \)

**Appendix B** Proofs for examples

**Proof of Proposition 7** The matrix of second derivatives of \( g(.) \) with respect to \( u \) is \( g^{(2)}(u) = h^{(2)}(u) + \Sigma^{-1} \), where \( h^{(2)}(u) \) is the matrix of second derivatives of \( h(.) \) with respect to \( u \), and \( h(.) \) is defined in (8). We have \( h^{(2)}(u) = Z^TW(u)Z \), where \( W(u) \) is a diagonal matrix with diagonal entries

\[
W_{ii}(u) = \frac{b''(X^T \beta + Z^T_i u)}{a_i(\beta)}.
\]
But \( a_i(\phi) > 0 \), and since \( b(.) \) is a convex function \( b''(X_i^T \beta + Z_i^T u) \geq 0 \), so \( W_i(u) \geq 0 \) for all \( u \). So \( W(u) \) is a non-negative definite matrix, and for any \( x \in \mathbb{R}^d \), \( x^T h^{(2)}(u)x = (xZ)^T W(Zx) \geq 0 \), which means that \( h^{(2)}(u) \) is non-negative definite. Since \( \Sigma^{-1} \) is positive definite, this means that \( g^{(2)}(u) \) is positive definite for all \( u \), so \( g(.) \) is strictly convex, and therefore has a unique minimum. Since \( b(.) \) is a smooth function, so is \( g(.) \), so Condition 4 holds. \( \square \)

**Proof of Proposition 3.** To prove the result, we need to show that after reparameterization Condition 2 holds with normalizing terms \( n_1, \ldots, n_d \), so that we can apply Theorem 1.

For \( k \geq 3 \), \( g^{(k)}(\cdot) \) is diagonal with diagonal terms \( g_{j,,j} = \Theta_p(n_j) \), so \( f^{(k)} = O^*_p(1) \) for \( k \geq 3 \). It remains to show that \( [f^{(2)}]^{-1} = O^*_p(1) \).

Write

\[
\Sigma_{jk}^{[l]} = \begin{cases} 
\sigma_1^2 + \sigma_2^2 + \ldots + \sigma_l^2 & \text{if } j = k \\
\sigma_2^2 + \ldots + \sigma_l^2 & \text{if } j \neq k, \text{ but } c_3(j) = c_3(k) \\
\vdots & \vdots \\
\sigma_l^2 & \text{if } c_{l-1}(j) \neq c_{l-1}(k), \text{ but } c_l(j) = c_l(k),
\end{cases}
\]

so that \( \Sigma = \Sigma^{[l]} \).

\( \Sigma^{[l]} \) is a block-diagonal matrix, with \( d_l \) blocks, one for each level-\( l \) cluster. We have

\[
\Sigma_{jk}^{[l]} = \begin{cases} 
\Sigma_{jk}^{[l-1]} + \sigma_l^2 & \text{if } c_l(j) = c_l(k) \\
0 & \text{otherwise}
\end{cases}
\]

Write \( \Sigma_{jk}^{[l]} = (\Sigma^{[l]}_{jk})^{-1} \). Applying the Sherman–Morrison formula to invert each block of \( \Sigma^{[l]} \) gives

\[
\Sigma_{jk}^{[l]} = \begin{cases} 
\Sigma_{jk}^{[l-1]} - \frac{\sigma_l^2 r_j r_k}{1 + \sigma_l^2 s_{c_l(j)}} & \text{if } c_l(j) = c_l(k) \\
0 & \text{otherwise}
\end{cases}
\]

where

\[
r_j = \sum_{k: c_k(j)=c_l(j)} \Sigma_{jk}^{[l-1]}, \quad s_c = \sum_{j: c(j)=c} r_j.
\]

We hypothesize that

\[
\Sigma_{jk}^{[l]} = \begin{cases} 
\Theta(1) & \text{if } j = k \\
\Theta((d_{c_l(j)})^{-1}) & \text{if } j \neq k, \text{ but } c_3(j) = c_3(k) \\
\vdots & \vdots \\
\Theta((d_{c_l(j)})^{-1}) & \text{if } c_{l-1}(j) \neq c_{l-1}(k), \text{ but } c_l(j) = c_l(k) \\
0 & \text{otherwise}
\end{cases}
\]

and prove this by induction on \( l \). This claim is true for \( l = 2 \), as \( \Sigma_{jk}^{[2]} = \sigma_2^{-2}I \).

For \( l \geq 2 \), applying the induction hypothesis to \( \Sigma_{jk}^{[l]} \), we find \( r_j = \Theta(1) \), so \( s_c = \Theta(d_c^{-1}) \) and

\[
\frac{\sigma_l^2 r_j r_k}{1 + \sigma_l^2 s_{c_l(j)}} = \Theta((d_c^{-1})^{-1}).
\]
Substituting (16) into (13) proves (15).

Now write $g[i][k] = h[i][k] - \Sigma[j][k]$, so that $g[j][k] = g[j][k]$. Again, $g[i]$ is block-diagonal, and

$$
g[i][k] = g[i][k] = \left(\Sigma[j][k] - \Sigma[i][k]\right)$$

$$
= \begin{cases} 
    g[i][k] + \frac{\sigma^2 r[j] r[k]}{1 + \sigma^2 s_c(j)} & \text{if } c_l(j) = c_l(k) \\
    0 & \text{otherwise.}
\end{cases}
$$

Write $g[i][k] = (g[i][k])^{-1}$. Applying the Sherman–Morrison formula to invert each block of $g[i]$ gives

$$
g[i][k] = \begin{cases} 
    g[i][k] - \frac{\alpha_j a_k}{1 + \alpha_j b_c(j)} & \text{if } c_l(j) = c_l(k) \\
    0 & \text{otherwise},
\end{cases}
$$

(17)

where

$$
\alpha = \frac{\sigma^2}{1 + \sigma^2 s_c(j)} = \Theta((d_l^j)^{-1}),
$$

$$
a_j = \sum_{k : c_l(k) = c_l(j)} r[j] g[i][k], \quad b_c = \sum_{j : c_l(j) = c_l(k) = c} r[j] g[i][k];
$$

(18)

We hypothesize that

$$
g[i][k] = \begin{cases} 
    O_p(n_j^{-1}) & \text{if } j = k \\
    O_p((d_l^{c_l(j)})^{-1} n_j^{-1} n_k^{-1}) & \text{if } j \neq k, \text{ but } c_l(j) = c_l(k) \\
    : & \\
    O_p((d_l^{c_l(j)})^{-1} n_j^{-1} n_k^{-1}) & \text{if } c_{l-1}(j) \neq c_{l-1}(k), \text{ but } c_l(j) = c_l(k) \\
    0 & \text{otherwise},
\end{cases}
$$

(19)

and prove this by induction on $l$. This claim is true for $l = 2$, as $g[2]$ is diagonal, with diagonal entries $h_{ij} + \sigma^2 = \Theta_p(n_j)$. For $l \geq 2$, applying the induction hypothesis to (18), recalling that $r[j] = \Theta(1)$, we find

$$
a_j = \sum_{k : c_{l(k)} = c_{l(j)}} O_p((d_l^{c_l(j)})^{-1} n_j^{-1} n_k^{-1}) = O_p(n_j^{-1})
$$

and

$$
b_c = \sum_{k : c_{l(k)} = c_{l(j)} = c} O_p((d_l^{c_l(j)})^{-1} n_j^{-1} n_k^{-1}) = O_p(1),
$$

so

$$
\frac{\alpha a_j a_k}{1 + \alpha b_c(j)} = \frac{a_j a_k}{\alpha^{-1} + b_c(j)} = O_p((d_l^{c_l(j)})^{-1} n_j^{-1} n_k^{-1})
$$

(20)

Substituting (20) into (17) proves (19).

Normalizing,

$$
f[i][k] = n_j^{-1/2} n_k^{-1/2} g[i][k] = n_j^{-1/2} n_k^{-1/2} g[i][k]
$$

$$
= \begin{cases} 
    O_p(1) & \text{if } j = k \\
    O_p((d_l^{c_l(j)})^{-1} n_j^{-1/2} n_k^{-1/2}) & \text{if } c_{l-1}(j) \neq c_{l-1}(k), \text{ but } c_l(j) = c_l(k), \\
    0 & \text{for } l = 3, \ldots, L
\end{cases}
$$

otherwise.
Then
\[
\sum_k |f^{jk}| = O_p \left( 1 + \sum_{l=3}^L \frac{\sum_{k, c_l(z(j)) \neq c_l(z(k))} (d^l_{c_l(z(j))})^{-1} n^{-1/2}}{n_k^{-1/2}} \right)
\]
\[
= O_p \left( 1 + \sum_{l=3}^L d^l_{c_l(z(j))} (d^l_{c_l(z(j))})^{-1} n^{-1/2} \max_k \{n_k^{-1/2}\} \right)
\]
\[
= O_p(1 + n^{-1/2}) = O_p(1),
\]
and \(\sum_j |f^{jk}| = \sum_k |f^{kj}| = O_p(1)\), so \(f^{(2)} = O_p^*(1)\). So Condition 2 holds with normalizing terms \(n_1, \ldots, n_d\), and Theorem 1 gives that \(\epsilon_k(\theta) = O_p(\sum_{j=1}^d n_j^{-k})\), as required.

References

Douglas Bates, Martin Mächler, Ben Bolker, and Steve Walker. Fitting linear mixed-effects models using lme4. *Journal of Statistical Software*, 67(1):1–48, 2015.

Randal Douc, Éric Moulines, and Tobias Rydén. Asymptotic properties of the maximum likelihood estimator in autoregressive models with Markov regime. *The Annals of Statistics*, 32(5):2254–2304, 2004.

P. McCullagh. *Tensor Methods in Statistics*, pages 254–256. Monographs on Statistics and Applied Probability. Chapman and Hall, 1987.

Lei Nie. Convergence rate of MLE in generalized linear and nonlinear mixed-effects models: Theory and applications. *Journal of Statistical Planning and Inference*, 137(6):1787–1804, 2007.

H. E. Ogden. On asymptotic validity of naive inference with an approximate likelihood. *Biometrika*, 104(1):153–164, 2017.

Stephen W. Raudenbush, Meng-Li Yang, and Matheos Yosef. Maximum likelihood for generalized linear models with nested random effects via high-order, multivariate Laplace approximation. *Journal of Computational and Graphical Statistics*, 9(1):141–157, 2000.

Håvard Rue, Sara Martino, and Nicolas Chopin. Approximate Bayesian inference for latent Gaussian models by using integrated nested Laplace approximations. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 71(2):319–392, 2009.

Zhenming Shun and Peter McCullagh. Laplace approximation of high dimensional integrals. *Journal of the Royal Statistical Society. Series B (Methodological)*, 57(4):749–760, 1995.

Christopher G Small. *Expansions and Asymptotics for Statistics*, chapter 6. Monographs on Statistics and Applied Probability. Chapman and Hall/CRC, 2010.

Vadim Zipunnikov and James G Booth. Closed form GLM cumulants and GLMM fitting with a SQUAR-EM-LA 2 algorithm, 2011.