

BOUNDS FOR THE CHI-SQUARE APPROXIMATION OF THE POWER DIVERGENCE FAMILY OF STATISTICS

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Abstract

It is well known that each statistic in the family of power divergence statistics, across n trials and r classifications with index parameter $\lambda \in \mathbb{R}$ (the Pearson, likelihood ratio, and Freeman–Tukey statistics correspond to $\lambda = 1, 0, -1/2$, respectively), is asymptotically chi-square distributed as the sample size tends to infinity. We obtain explicit bounds on this distributional approximation, measured using smooth test functions, that hold for a given finite sample n , and all index parameters ($\lambda > -1$) for which such finite-sample bounds are meaningful. We obtain bounds that are of the optimal order n^{-1} . The dependence of our bounds on the index parameter λ and the cell classification probabilities is also optimal, and the dependence on the number of cells is also respectable. Our bounds generalise, complement, and improve on recent results from the literature.

Keywords: Power divergence statistic; likelihood ratio statistic; Pearson’s statistic; chi-square approximation; rate of convergence; Stein’s method

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1. Introduction

Consider the setting of a multinomial goodness-of-fit test, with n independent trials in which each trial leads to a unique classification over $r \geq 2$ classes. Let U_1, \dots, U_r represent the observed frequencies arising in each class, and denote the non-zero classification probabilities by $\mathbf{p} = (p_1, \dots, p_r)$. In 1984, Cressie and Read [7] introduced the *power divergence family of statistics* for testing the null hypothesis $H_0: \mathbf{p} = \mathbf{p}_0$ against the alternative hypothesis $H_1: \mathbf{p} = \mathbf{p}_1$. These statistics are given by

$$T_\lambda = \frac{2}{\lambda(\lambda + 1)} \sum_{j=1}^r U_j \left[\left(\frac{U_j}{np_j} \right)^\lambda - 1 \right], \quad (1)$$

where the index parameter $\lambda \in \mathbb{R}$. Here, and throughout the paper, we assume the validity of the null hypothesis, and, for ease of notation, suppress the subscript in the notation \mathbf{p}_0 . Note that $\sum_{j=1}^r U_j = n$ and $\sum_{j=1}^r p_j = 1$.

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When $\lambda = 0, -1$, the notation in (1) should be understood as a result of passage to the limit, in which cases we recover the log-likelihood ratio and modified log likelihood ratio statistics, respectively:

$$L = 2 \sum_{j=1}^r U_j \log\left(\frac{U_j}{np_j}\right), \quad GM^2 = 2n \sum_{j=1}^r p_j \log\left(\frac{np_j}{U_j}\right). \tag{2}$$

The cases $\lambda = 1, -1/2$ correspond to Pearson’s chi-square statistic [25] and the Freeman–Tukey statistic [10], given by

$$\chi^2 = \sum_{j=1}^r \frac{(U_j - np_j)^2}{np_j}, \quad T^2 = 4 \sum_{j=1}^r (\sqrt{U_j} - \sqrt{np_j})^2. \tag{3}$$

The power divergence family of statistics can therefore be seen to unify several commonly used goodness-of-fit tests. The statistic $T_{2/3}$, often referred to as the Cressie–Read statistic, was also suggested in [7, 32] as a good alternative to the classical likelihood ratio and Pearson statistics.

A fundamental result is that, for all $\lambda \in \mathbb{R}$, the statistic T_λ converges in distribution to the $\chi^2_{(r-1)}$ distribution as the number of trials n tends to infinity [7, p. 443]. However, in practice we have a finite sample, and so it is of interest to assess the quality of this distributional approximation for finite n . In the literature, this has been done on the one hand through theoretical bounds on the rate of convergence, which will be the focus of this paper, and on the other through simulation studies. The findings of simulation studies from the literature are briefly reviewed in Remark 4, in which we also discuss how the theoretical bounds obtained in this paper reflect the findings of these studies.

From the theoretical literature, the quality of the chi-square approximation of the distribution of the statistic T_λ has been assessed by Edgeworth expansions [3, 4, 11, 29, 31, 37]. In [31], Edgeworth expansions were used to propose closer approximations to the distribution function of T_λ that are of the form of the $\chi^2_{(r-1)}$ distribution function plus an $o(1)$ correction. The work of [31] generalised results of [34] that had been given for the Pearson, likelihood ratio, and Freeman–Tukey statistics ($\lambda = 1, 0, -1/2$). However, as noted in [29], it is impossible to determine a rate of convergence from the expansions given in [31, 34]. Bounds on the rate of convergence of the distribution of T_λ to its limiting $\chi^2_{(r-1)}$ distribution via Edgeworth expansions were obtained in [11, 29]. For $r \geq 4$, [37] obtained an $O(n^{-(r-1)/r})$ bound on the rate of convergence in the Kolmogorov distance (see also [3] for a refinement of this result) and, for $r = 3$, [4] obtained an $O(n^{-3/4+0.065})$ bound on the rate of convergence in the same metric, with both bounds holding for all $\lambda \in \mathbb{R}$.

Bounds on the rate of convergence have also been given for special cases of the power divergence family. For the likelihood ratio statistic, [2] recently used Stein’s method to obtain an explicit $O(n^{-1/2})$ bound for smooth test functions. It is worth noting that the setting of [2] was more general than the categorical data setting of this paper. For Pearson’s statistic, it was shown in [38] using Edgeworth expansions that a bound on the rate of convergence of Pearson’s statistic in the Kolmogorov distance is $O(n^{-(r-1)/r})$ for $r \geq 2$, which was improved by [17] to $O(n^{-1})$ for $r \geq 6$. An explicit $O(n^{-1/2})$ Kolmogorov distance bound was obtained by Stein’s method in [22]. Recently, [14] used Stein’s method to obtain explicit error bounds for Pearson’s statistic, measured using smooth test functions. These bounds will be needed in the following, and are recorded here.

Let $C_b^k(\mathbb{R}^+)$ denote the class of bounded functions $h : \mathbb{R}^+ \rightarrow \mathbb{R}$ for which $h^{(k)}$ exists and derivatives up to k th order are bounded. Let $r \geq 2$ and $p_* := \min_{1 \leq j \leq r} p_j$. Suppose $np_* \geq 1$. Then, the following bounds were obtained in [14]. For $h \in C_b^5(\mathbb{R}^+)$,

$$|\mathbb{E}[h(\chi^2)] - \chi_{(r-1)}^2 h| \leq \frac{4}{(r+1)n} \left(\sum_{j=1}^r \frac{1}{\sqrt{p_j}} \right)^2 \{19\|h\| + 366\|h'\| + 2016\|h''\| + 5264\|h^{(3)}\| + 106\,965\|h^{(4)}\| + 302\,922\|h^{(5)}\|\}, \tag{4}$$

and, for $h \in C_b^2(\mathbb{R}^+)$,

$$|\mathbb{E}[h(\chi^2)] - \chi_{(r-1)}^2 h| \leq \frac{24}{(r+1)\sqrt{n}} \{3\|h\| + 23\|h'\| + 42\|h''\|\} \sum_{j=1}^r \frac{1}{\sqrt{p_j}}, \tag{5}$$

where $\chi_{(r-1)}^2 h$ denotes the expectation $\mathbb{E}[h(Y_{r-1})]$ for $Y_{r-1} \sim \chi_{(r-1)}^2$. Here and throughout the paper, we write $\|\cdot\|$ for the usual supremum norm $\|\cdot\|_\infty$ of a real-valued function. The bound in (4) achieves the optimal $O(n^{-1})$ rate, although when the constants are large compared to n the bound in (5) may give the smaller numerical bound. Both bounds (4) and (5) have an optimal dependence on p_* , since, for a fixed number of classes r , both bounds tend to zero if and only if $np_* \rightarrow \infty$, which is precisely the condition under which $\chi^2 \rightarrow_d \chi_{(r-1)}^2$ (see [18]). The bounds (4) and (5) are the first in the literature on Pearson’s statistic to decay to zero if and only if $np_* \rightarrow \infty$, and in the case of (4) achieve the optimal $O(n^{-1})$ rate for all $r \geq 2$.

In this paper, we generalise the bounds of [14] to the family of power divergence statistics T_λ , $\lambda > -1$, the largest subclass of the power divergence family for which finite-sample bounds can be given when measured using smooth test functions, as in (4) and (5). Indeed, it can be seen from (1) and (2) that, for $\lambda \leq -1$, we have $T_\lambda = \infty$ if any of the observed frequencies U_1, \dots, U_r are zero, meaning that the expectation $\mathbb{E}[h(T_\lambda)]$ is undefined. The bounds in Theorem 2 are of the optimal n^{-1} order. Specialising to the case $\lambda = 0$ of the likelihood ratio statistic, our $O(n^{-1})$ bound improves on the $O(n^{-1/2})$ rate (and has a better dependence on the other model parameters) of [2] that was given in a more general setting than that of the categorical data considered in this paper. Our results also complement [15] in which Stein’s method is used to obtain order $O(n^{-1})$ bounds for the chi-square approximation of Friedman’s statistic. In Theorem 3, we provide suboptimal $O(n^{-1/2})$ bounds which may yield smaller numerical bounds for small sample sizes n .

Like the bounds of [14] for Pearson’s statistic, for all fixed $\lambda > -1$ and $r \geq 2$, the bounds of Theorems 2 and 3 enjoy the property of decaying to zero if and only if $np_* \rightarrow \infty$. If $r \geq 2$ is fixed and we allow λ to vary with n , then the bounds of Theorems 2 and 3 tend to zero if and only if $np_*/\lambda^2 \rightarrow \infty$, which is again an optimal condition (see Remark 3). The dependence of our bounds on r is also respectable. The excellent dependence of the bounds of Theorem 3 on all parameters allows us to prescribe simple conditions under which the chi-square approximation is valid, when the quantities λ , r , and p_1, \dots, p_r may vary with n ; see Remark 3. As already discussed, some of these conditions are optimal, and in parameter regimes in which we have not been able to obtain optimal conditions we conjecture what these optimal conditions are; see Remark 3, again.

It is perhaps not a priori obvious that the $O(n^{-1})$ rate of our main bounds would hold for all power divergence statistics with $\lambda > -1$. For example, simulation studies have shown that for small samples n the likelihood ratio statistic ($\lambda = 0$) is less accurate at approximating the limiting $\chi_{(r-1)}^2$ distribution than is Pearson’s statistic ($\lambda = 1$; see, for example, [5, 20]).

Our results show, however, that at least when measured using smooth test functions, the actual rate of convergence is the same for large n if the number of classes r is fixed. If the number of classes r is allowed to grow with n , then Pearson’s statistic will converge faster, though (see Remark 3). It is also important to note that our assumption of smooth test functions is essential for the purpose of obtaining $O(n^{-1})$ convergence rates that hold for all $r \geq 2$ and all $\lambda > -1$. For example, in the case $r = 3$, convergence rates in the Kolmogorov metric can be no faster than $O(n^{-3/4} \log \log n)$; see [4, Remark 3].

The rest of the paper is organised as follows. In Section 2 we state our main results. Theorem 1 provides analogues of the bounds (4) and (5) for Pearson’s statistic that hold for wider classes of test functions at the expense of a worse dependence on the parameter r . Our main result, Theorem 2, provides $O(n^{-1})$ bounds to quantify the chi-square approximation of the power divergence statistics. Alternative $O(n^{-1/2})$ bounds are given in Theorem 3, and from one of these bounds we extract a Kolmogorov distance bound (Corollary 1). We end Section 2 with several remarks discussing the bounds. In Section 3, we present several preliminary lemmas that are needed for the proofs of our main results. We prove the main results in Section 4. In Appendix A we present some basics of Stein’s method for chi-square approximation and use it to give a short proof of Theorem 1. Finally, in Appendix B we prove a technical lemma from Section 3.

2. Main results

We first present a theorem which complements the main result of [14] by giving explicit error bounds for the chi-square approximation of Pearson’s statistic that hold for larger classes of function than those used by [14]. The proof involves a minor modification of the proof of the bounds (4) and (5) of [14], and the details are given in Appendix A.

Before stating the theorem, we introduce some notation. We let $p_* := \min_{1 \leq j \leq r} p_j$. Let $C_b^{j,k}(\mathbb{R}^+)$, $j \leq k$, denote the class of functions $h : \mathbb{R}^+ \rightarrow \mathbb{R}$ for which $h^{(k)}$ exists and derivatives of order $j, j + 1, \dots, k$ are bounded. Note that $C_b^k(\mathbb{R}^+) \subset C_b^{j,k}(\mathbb{R}^+)$ for $j \geq 1$.

Theorem 1. *Let (U_1, \dots, U_r) be the multinomial vector of n observed counts, where $r \geq 2$, and suppose that $np_* \geq 1$. Let χ^2 be Pearson’s chi-square statistic as defined in (3). Then, for $h \in C_b^{1,5}(\mathbb{R}^+)$,*

$$|\mathbb{E}[h(\chi^2)] - \chi_{(r-1)}^2 h| \leq \frac{1}{(r+1)^{1/2} n} \left(\sum_{j=1}^r \frac{1}{\sqrt{p_j}} \right)^2 \left\{ 122 \|h'\| + 1970 \|h''\| + 6943 \|h^{(3)}\| + 12\,731 \|h^{(4)}\| + 643\,710 \|h^{(5)}\| \right\}, \tag{6}$$

and, for $h \in C_b^{1,2}(\mathbb{R}^+)$,

$$|\mathbb{E}[h(\chi^2)] - \chi_{(r-1)}^2 h| \leq \frac{1}{\sqrt{(r+1)n}} \{ 115 \|h'\| + 536 \|h''\| \} \sum_{j=1}^r \frac{1}{\sqrt{p_j}}. \tag{7}$$

Also, for $h \in C_b^{2,5}(\mathbb{R}^+)$,

$$|\mathbb{E}[h(\chi^2)] - \chi_{(r-1)}^2 h| \leq \frac{1}{n} \left(\sum_{j=1}^r \frac{1}{\sqrt{p_j}} \right)^2 \left\{ 19 \|h''\| + 206 \|h^{(3)}\| + 545 \|h^{(4)}\| + 161\,348 \|h^{(5)}\| \right\}, \tag{8}$$

and, for $h \in C_b^{2,2}(\mathbb{R}^+)$,

$$|\mathbb{E}[h(\chi^2)] - \chi_{(r-1)}^2 h| \leq \frac{238 \|h''\|}{\sqrt{n}} \sum_{j=1}^r \frac{1}{\sqrt{p_j}}. \tag{9}$$

The following weak convergence theorem for smooth test functions with a bound of order n^{-1} for the $\chi_{(r-1)}^2$ approximation of the power divergence statistic T_λ (which holds for all $\lambda > -1$ and $r \geq 2$) is the main result of this paper.

Theorem 2. Let (U_1, \dots, U_r) represent the multinomial vector of n observed counts, where $r \geq 2$. For $\lambda > -1$, let T_λ be the power divergence statistic as defined in (1). Suppose that $np_* \geq r$. If $\lambda \geq 3$, we also suppose that $np_* \geq 2(\lambda - 3)^2$. Then, for $h \in C_b^5(\mathbb{R}^+)$,

$$\begin{aligned} |\mathbb{E}[h(T_\lambda)] - \chi_{(r-1)}^2 h| \leq & \frac{1}{n} \left(\sum_{j=1}^r \frac{1}{p_j} \right) \left\{ \frac{4r}{r+1} \{19 \|h\| + 366 \|h'\| + 2016 \|h''\| \right. \\ & + 5264 \|h^{(3)}\| + 106\,965 \|h^{(4)}\| + 302\,922 \|h^{(5)}\| \} \\ & + |\lambda - 1| r \{2 \|h'\| + 202 \|h''\| + 819 \|h^{(3)}\| + 100\,974 \|h^{(4)}\| \} \\ & + \frac{19}{9} (\lambda - 1)^2 \|h''\| + \frac{|(\lambda - 1)(\lambda - 2)|(12\lambda + 13)}{6(\lambda + 1)} \|h'\| \}. \end{aligned} \tag{10}$$

Also, under the weaker assumption that $h \in C_b^{1,5}(\mathbb{R}^+)$,

$$\begin{aligned} |\mathbb{E}[h(T_\lambda)] - \chi_{(r-1)}^2 h| \leq & \frac{1}{n} \left(\sum_{j=1}^r \frac{1}{p_j} \right) \left\{ \frac{r}{\sqrt{r+1}} \{122 \|h'\| + 1970 \|h''\| \right. \\ & + 6943 \|h^{(3)}\| + 12\,731 \|h^{(4)}\| + 643\,710 \|h^{(5)}\| \} \\ & + |\lambda - 1| r \{2 \|h'\| + 202 \|h''\| + 819 \|h^{(3)}\| + 100\,974 \|h^{(4)}\| \} \\ & + \frac{19}{9} (\lambda - 1)^2 \|h''\| + \frac{|(\lambda - 1)(\lambda - 2)|(12\lambda + 13)}{6(\lambda + 1)} \|h'\| \}. \end{aligned} \tag{11}$$

If the constants are large compared to n , the next result may give smaller numerical bounds.

Theorem 3. Let $\lambda > -1$, $r \geq 2$, and $np_* \geq 2$. If $\lambda \geq 2$, we also suppose that $np_* \geq 2(\lambda - 2)^2$. Then, for $h \in C_b^2(\mathbb{R}^+)$,

$$\begin{aligned} |\mathbb{E}[h(T_\lambda)] - \chi_{(r-1)}^2 h| \\ \leq \left(\frac{24}{r+1} \{3 \|h\| + 23 \|h'\| + 42 \|h''\|\} + \frac{|\lambda - 1|(4\lambda + 7)}{\lambda + 1} \|h'\| \right) \sum_{j=1}^r \frac{1}{\sqrt{np_j}}. \end{aligned} \tag{12}$$

Also, under the weaker assumption that $h \in C_b^{1,2}(\mathbb{R}^+)$,

$$\begin{aligned} |\mathbb{E}[h(T_\lambda)] - \chi_{(r-1)}^2 h| \\ \leq \left(\frac{1}{\sqrt{r+1}} \{115 \|h'\| + 536 \|h''\|\} + \frac{|\lambda - 1|(4\lambda + 7)}{\lambda + 1} \|h'\| \right) \sum_{j=1}^r \frac{1}{\sqrt{np_j}}. \end{aligned} \tag{13}$$

In the following corollary we deduce a Kolmogorov distance bound from (12) by applying a basic technique (see [6, p. 48]) for converting smooth test function bounds into Kolmogorov distance bounds. As this technique is fairly crude, our resulting bound has a suboptimal dependence on n , although it does inherit the desirable property of decaying to zero if and only if $np_* \rightarrow \infty$, for fixed r and λ . This is the first Kolmogorov distance bound for the chi-square approximation of the statistic T_λ to enjoy this property.

Corollary 1. *Let $\lambda > -1$, $r \geq 2$. and $np_* \geq 2$. If $\lambda \geq 2$, we additionally suppose that $np_* \geq 2(\lambda - 2)^2$. Also, let $Y_{r-1} \sim \chi^2_{(r-1)}$. Then*

$$\sup_{z>0} |\mathbb{P}(T_\lambda \leq z) - \mathbb{P}(Y_{r-1} \leq z)| \leq \begin{cases} \frac{1}{(np_*)^{1/10}} \left\{ 8 + \left(21 + \frac{|\lambda - 1|(4\lambda + 7)r}{52(\lambda + 1)} \right) \frac{1}{(np_*)^{1/5}} + \frac{72}{(np_*)^{2/5}} \right\}, & r = 2, \\ \frac{1}{(np_*)^{1/6}} \left\{ 19 + \left(44 + \frac{|\lambda - 1|(4\lambda + 7)r}{25(\lambda + 1)} \right) \frac{1}{(np_*)^{1/6}} + \frac{72}{(np_*)^{1/3}} \right\}, & r = 3, \\ \frac{1}{(r - 3)^{1/3}(np_*)^{1/6}} \left\{ 13 + \left(37 + \frac{|\lambda - 1|(4\lambda + 7)r}{30(\lambda + 1)} \right) \frac{(r - 3)^{1/6}}{(np_*)^{1/6}} + \frac{72(r - 3)^{1/3}}{(np_*)^{1/3}} \right\}, & r \geq 4. \end{cases}$$

Remark 1. (On the proofs and assumptions.) Our proofs of Theorems 2 and 3 involve writing the power divergence statistic T_λ in the form $T_\lambda = \chi^2 + R$, where R is a ‘small’ remainder term. By this approach, to obtain our bounds on the quantity of interest $|\mathbb{E}[h(T_\lambda)] - \chi^2_{(r-1)}h|$, we make use of the bounds on $|\mathbb{E}[h(\chi^2)] - \chi^2_{(r-1)}h|$ given by (4)–(7). In the case $\lambda = 1$, $T_\lambda = \chi^2$, meaning that $R = 0$, which explains why our bounds reduce almost exactly to those bounds when $\lambda = 1$, with the only difference being that at the end of our proof of Theorem 2 we use the inequality $(\sum_{j=1}^r p_j^{-1/2})^2 \leq r \sum_{j=1}^r p_j^{-1}$ to obtain a compact final bound.

Our approach of decomposing $T_\lambda = \chi^2 + R$ means that we inherit large numerical constants from the bounds (4)–(7). However, as was the case in [14], our primary concern is simple final bounds with good dependence on the parameters n , λ , r , and p_1, \dots, p_r . In proving Theorems 2 and 3, we make some crude approximations but take care to ensure they do not affect the role of the parameters in the final bound.

In order to simplify the calculations and arrive at our desired compact final bounds, we made some assumptions. We discuss here the assumptions for Theorem 2; similar comments apply to the assumptions of Theorem 3. The assumption $np_* \geq r$ ($\lambda \neq 1$), $np_* \geq 1$ ($\lambda = 1$) is very mild (the bounds in Theorem 2 are uninformative otherwise) and was made for the purpose of simplifying the calculations and to allow us to obtain a compact final bound (it allows the bound of Lemma 3 to be given in a compact form). This assumption is also natural, because we require that $np_*/r \rightarrow \infty$ in order for $T_\lambda \rightarrow_d \chi^2_{(r-1)}$ (see Remark 3). The assumption $np_* \geq 2(\lambda - 3)^2$, $\lambda \geq 3$, is also mild (our bound cannot be small unless this condition is met) and natural because a necessary condition for $T_\lambda \rightarrow_d \chi^2_{(r-1)}$ is that $np_*/\lambda^2 \rightarrow \infty$ (see Remark 3). This assumption is needed to apply Lemma 2 and, again, is useful in allowing a compact bound to be given.

Remark 2. (*The class of functions and integral probability metrics (IPMs).*) The bound (10) of Theorem 2 is in a sense preferable to the bound (11) because in the case $\lambda = 1$ it has a better dependence on r . However, an advantage of the bound (11) is that it holds for a wider class of test functions h while having the same dependence on all parameters $n, \lambda, r,$ and p_1, \dots, p_r if $\lambda \neq 1$. We now see how this advantage plays out if the smooth test function bounds are converted into bounds involving integral probability metrics.

The bounds of Theorems 1–3 can be expressed in terms of convergence determining IPMs [16, 39] as follows. Let $\mathcal{H}_{q_1, q_2} = \{h \in C_b^{q_1, q_2}(\mathbb{R}^+) : \|h^{(q_1)}\| \leq 1, \|h^{(q_1+1)}\| \leq 1, \dots, \|h^{(q_2-1)}\| \leq 1, \|h^{(q_2)}\| \leq 1\}$, where $h^{(0)} \equiv h$. Then we define the IPM between the laws of real-valued random variables X and Y by $d_{q_1, q_2}(\mathcal{L}(X), \mathcal{L}(Y)) = \sup_{h \in \mathcal{H}_{q_1, q_2}} |\mathbb{E}[h(X)] - \mathbb{E}[h(Y)]|$. As an example, for $Y_{r-1} \sim \chi_{(r-1)}^2$, from (11) we obtain the two-sided inequality

$$|\mathbb{E}[T_\lambda] - \mathbb{E}[Y_{r-1}]| \leq d_{1,5}(\mathcal{L}(T_\lambda), \chi_{(r-1)}^2) \leq \frac{1}{n} \left(\sum_{j=1}^r \frac{1}{p_j} \right) \left\{ 665\,476\sqrt{r} + 101\,997|\lambda - 1|r + \frac{19}{9}(\lambda - 1)^2 + \frac{|\lambda - 1|(\lambda - 2)(12\lambda + 13)}{6(\lambda + 1)} \right\}, \quad (14)$$

where the lower bound follows because $h(x) = x$ is in the class $\mathcal{H}_{1,5}$. If $r \geq 2$, then $\mathbb{E}[T_1] = \mathbb{E}[\chi^2] = \mathbb{E}[Y_{r-1}]$, and it was shown in [7, p. 451] (here we have written their formula in a slightly different form) that, for $\lambda > -1$,

$$|\mathbb{E}[T_\lambda] - \mathbb{E}[Y_{r-1}]| = \left| \sum_{j=1}^r \left\{ \frac{(\lambda - 1)}{np_j} \left[\frac{3\lambda - 2}{12} - \frac{\lambda p_j}{2} + \frac{3\lambda + 2}{12} p_j^2 \right] \right\} + O(n^{-3/2}) \right|. \quad (15)$$

It should be noted that $\mathbb{E}[T_{-1}] = \infty$, and that the $O(n^{-3/2})$ term in the asymptotic approximation for $|\mathbb{E}[T_\lambda] - \mathbb{E}[Y_{r-1}]|$ therefore blows up as $\lambda \downarrow -1$. We also note that comparing the lower and upper bounds in (14) shows that the upper bound (14) has a good dependence on all parameters, $n, \lambda, r,$ and p_1, \dots, p_r . This is the subject of the next remark.

Remark 3. (*The dependence of the bounds on the parameters and conditions for convergence.*) A basic necessary condition for T_λ to converge in distribution to $\chi_{(r-1)}^2$ is that $\mathbb{E}[T_\lambda] \rightarrow \mathbb{E}[Y_{r-1}]$ for $Y_{r-1} \sim \chi_{(r-1)}^2$. Therefore, we can study the optimality of the bounds of Theorems 2 and 3 on the parameters $n, \lambda, r,$ and p_1, \dots, p_r via comparison with the asymptotic approximation in (15). We observe that the $O(n^{-1})$ rate of convergence of the upper bounds in Theorem 2 is optimal. Moreover, the dependence on p_* of the form $(np_*)^{-1}$ is also the best possible, as is the dependence on λ of the form λ^2/n for large n and λ . The bounds in Theorem 3 are of the suboptimal order $O(n^{-1/2})$, but otherwise also have the correct dependence on p_* and λ , because they tend to zero if and only if $np_* \rightarrow \infty$ (with fixed r and λ) and $n/\lambda^2 \rightarrow \infty$ (with fixed r and p_*).

Let us now consider the dependence of the bounds of Theorems 2 and 3 on r . To do this, we consider the case of uniform cell classification probabilities, $p_1 = \dots = p_r = 1/r$, and suppose $\lambda \neq 1$ is fixed. Then, for large r , $|\mathbb{E}[T_\lambda] - \mathbb{E}[Y_{r-1}]| \rightarrow 0$ if and only if $n/r^2 \rightarrow \infty$, except when $\lambda = 2/3$, in which case $|\mathbb{E}[T_{2/3}] - \mathbb{E}[Y_{r-1}]| \rightarrow 0$ if and only if $n/r \rightarrow \infty$. In this case of uniform cell classification probabilities, the bounds of Theorems 2 and 3 converge to zero, for fixed $\lambda \neq 1$, if and only if $n/r^3 \rightarrow \infty$. We consider it most likely that $T_\lambda \rightarrow_d \chi_{(r-1)}^2$ if $n/r^2 \rightarrow \infty$, and that our bounds therefore do not have an optimal dependence on r . In the

proof of Theorem 2, our bounds for all the remainder terms except R_3 decay to zero if and only if $n/r^2 \rightarrow \infty$, while our bound for R_3 decays to zero if and only if $n/r^3 \rightarrow \infty$. The bound for R_3 follows from a long calculation involving analysis of the multivariate normal Stein equation; see Part II of the proof of [14, Theorem 4.2]. It is plausible that a more refined analysis could lead to a bound for R_3 with an improved dependence on r . We consider this to be an interesting but challenging problem.

If we consider the possibility that, as $n \rightarrow \infty$, p_* may decay to zero, $\lambda \neq 1$, and r may tend to infinity, we can read off from the upper bounds of Theorem 2 that $T_\lambda \rightarrow_d \chi^2_{(r-1)}$ if $n/(S\lambda \max\{r, \lambda\}) \rightarrow \infty$, where $S = \sum_{j=1}^r p_j^{-1}$. If we suppose that $r/\lambda \rightarrow c$, where $0 \leq c < \infty$, then we see that $T_\lambda \rightarrow_d \chi^2_{(r-1)}$ if $n/(S\lambda^2) \rightarrow \infty$. From (15) this can be seen to be an optimal condition (except perhaps if $\lambda = 2/3$). We conjecture that in fact $T_\lambda \rightarrow_d \chi^2_{(r-1)}$ if $n/(S\lambda^2) \rightarrow \infty$, even if $r \gg \lambda$ (except perhaps if $\lambda = 2/3$).

In stating the above conditions we have been careful to give them in terms of the sum S rather than p_* , because in the $r \rightarrow \infty$ regime it is possible that $S \ll r/p_*$. For example, take $p_1 = n^{-1}$, $p_j = (n-1)/(n(r-1))$, $j = 2, \dots, r$, so that $\sum_{j=1}^r p_j = 1$. Then $S = n + (r-1)^2 n/(n-1) \ll rn = r/p_*$ if $r \ll n$. If, however, $r/(p_* S) \rightarrow C$, where $1 \leq C < \infty$ (which will be the case unless there are some exceptionally small cell classification probabilities), then we can write the conditions in a simple and intuitive form by replacing S by r/p_* . For example, our conjectured optimal condition for which $T_\lambda \rightarrow_d \chi^2_{(r-1)}$ would read $np_*/(r\lambda^2) \rightarrow \infty$.

From (5) we see that, even if $r \rightarrow \infty$, $T_1 = \chi^2 \rightarrow_d \chi^2_{(r-1)}$ provided $np_* \rightarrow \infty$, which is a well-established condition for chi-square approximation of Pearson’s statistic to be valid (see [18]). Thus, in the $r \rightarrow \infty$ regime, it can be seen that Pearson’s statistic converges in distribution faster than any other member of the power divergence family, except perhaps $T_{2/3}$ for which we are unable to provide a definitive answer in this paper.

Remark 4. (*Comparison to results from simulation studies.*) Simulation studies assessing the quality of chi-square approximation of the statistic T_λ can be found in, amongst others, [7, 23, 30, 32, 33]. In this remark we show how some of the findings of these studies are reflected in our bounds. As is common with small-sample studies for goodness-of-fit tests, most of the studies assumed that the classification probabilities are uniform ($p_j = 1/r$ for all $j = 1, \dots, r$) [19, p. 339]. Under this assumption, [30] concluded that, for $\lambda \in [1/3, 3/2]$, the chi-square approximation of T_λ is accurate for the purpose of hypothesis testing at significance levels between 0.1 and 0.01, provided $r \leq 6$ and $n \geq 10$ [that the approximation can be accurate for sample sizes as small as $n = 10$ is consistent with the fast $O(n^{-1})$ rate of convergence of the bounds of Theorem 2]. However, if $|\lambda|$ increases, the approximation becomes worse, and this is magnified as r increases for fixed n [our bounds grow as λ and r increase]. Outside the equiprobable hypothesis, it is harder to prescribe general rules [19, p. 341], although the accuracy of the approximation diminishes [26] [as we move away from the equiprobable hypothesis the sum $\sum_{j=1}^r p_j^{-1}$ increases].

Through a combination of simulation studies and theoretical considerations, [7] proposed the statistic $T_{2/3}$ as an alternative to the classical likelihood ratio and Pearson statistics. One of the reasons was because they observed that for the quantities $\mathbb{E}[T_\lambda^k] - \mathbb{E}[Y_{r-1}^k]$, $k = 1, 2, 3$, for $Y_{r-1} \sim \chi^2_{(r-1)}$, the second-order correction terms vanish in the limit $r \rightarrow \infty$ if and only if $\lambda = 2/3, 1$. Our bounds do converge faster in the case $r \rightarrow \infty$ if $\lambda = 1$, but not if $\lambda = 2/3$, and we know that for $\lambda \in (-1, \infty) \setminus \{2/3, 1\}$ the true convergence rate is indeed slower in this regime. It would be interesting to provide a definitive answer as to whether the convergence

rate does speed up in the large- r regime if $\lambda = 2/3$. We do, however, note that in our method of proof there seems to be nothing special about the case $\lambda = 2/3$, so a different approach would be required to provide a positive answer.

3. Preliminary lemmas

We begin by presenting a series of moment bounds for binomial random variables.

Lemma 1. *Let $S = (U - np)/\sqrt{np}$, where $U \sim \text{Bin}(n, p)$, for $n \geq 1$, $0 < p < 1$ such that $np \geq 2$. Then*

$$\mathbb{E}[|S|^3] \leq 3, \tag{16}$$

$$\mathbb{E}[S^4] \leq 4, \tag{17}$$

$$\mathbb{E}[S^6] \leq 28. \tag{18}$$

Proof. Using standard formulas for the fourth and sixth central moments of the binomial distribution (see, for example [36]), we have that

$$\mathbb{E}[S^4] = \frac{1}{(np)^2} \cdot np(1-p)[3(2-n)p^2 + 3(n-2)p + 1] \leq 3 + \frac{1}{np} \leq \frac{7}{2} < 4$$

and

$$\begin{aligned} \mathbb{E}[S^6] &= \frac{1}{(np)^3} \cdot np(1-p)[5(3n^2 - 26n + 24)p^4 - 10(3n^2 - 26n + 24)p^3 \\ &\quad + 5(3n^2 - 31n + 30)p^2 + 5(5n - 6)p + 1] \leq 15 + \frac{25}{np} + \frac{1}{(np)^2} < 28, \end{aligned}$$

where we used that $n \geq 1$, $0 < p < 1$, and $np \geq 2$ to simplify the bounds. Inequality (16) follows from (17) by Hölder’s inequality: $\mathbb{E}[|S|^3] \leq (\mathbb{E}[S^4])^{3/4} \leq 4^{3/4} < 3$. □

Lemma 2. (T. D. Ahle [1].) *Let $U \sim \text{Bin}(n, p)$, where $n \geq 1$ and $0 < p < 1$. Let $k > 0$. Then $\mathbb{E}[U^k] \leq \exp(k^2/(2np)) \cdot (np)^k$. Suppose now that $np \geq \alpha k^2$, where $\alpha > 0$. Then it is immediate from the previous expression that*

$$\mathbb{E}[U^k] \leq e^{1/(2\alpha)}(np)^k. \tag{19}$$

Remark 5. Bounds of the form $\mathbb{E}[U^k] \leq C_k(np)^k$, where C_k is an explicit constant only depending on k , in which there are no further restrictions on n and p , are available (see [28]). However, for our purpose of obtaining bounds with the best possible dependence on all parameters, such a bound is not suitable, as it would lead to a worse dependence on λ in the final bound. The additional assumption $np \geq \alpha k^2$ for inequality (19) leads to the assumption $np \geq 2(\lambda - 3)^2$, $\lambda \geq 3$, in Theorem 2 (and a similar assumption in Theorem 3), which is mild and preferable to a worse dependence of the bounds on λ .

Lemma 3. *Let (U_1, \dots, U_r) be the multinomial vector of observed counts, as in Theorem 2, where $r \geq 2$. Suppose also that $np_j \geq r$ for all $j = 1, \dots, r$. For $j = 1, \dots, r$, let $S_j = (U_j - np_j)/\sqrt{np_j}$. Then, for $j \neq k$,*

$$|\mathbb{E}[S_j^3 S_k^3]| \leq \frac{6}{r} + 4\sqrt{p_j p_k}. \tag{20}$$

Proof. Let $I_j(i)$ be the indicator that trial i results in classification in cell j , and let $\tilde{I}_j(i) = I_j(i) - p_j$ be its standardised version. We can then write $S_j = (np_j)^{-1/2} \sum_{i=1}^n \tilde{I}_j(i)$. We note that $\tilde{I}_{j_1}(i_1)$ and $\tilde{I}_{j_2}(i_2)$ are independent for all $j_1, j_2 \in \{1, \dots, r\}$ if $i_1 \neq i_2$. On using this property together with the fact that $\mathbb{E}[\tilde{I}_j(i)] = 0$ for all $i = 1, \dots, n$ and $j = 1, \dots, r$, we obtain that, for $j \neq k$,

$$\begin{aligned} \mathbb{E}[S_j^3 S_k^3] &= \frac{1}{n^3(p_j p_k)^{3/2}} \mathbb{E} \left[\left(\sum_{i=1}^n \tilde{I}_j(i) \right)^3 \left(\sum_{\ell=1}^n \tilde{I}_k(\ell) \right)^3 \right] \\ &= \frac{1}{n^3(p_j p_k)^{3/2}} \left\{ \sum_{i_1=1}^n \mathbb{E}[\tilde{I}_j(i_1)^3 \tilde{I}_k(i_1)^3] + \sum_{i_1=1}^n \sum_{i_2 \neq i_1}^n \left\{ \mathbb{E}[\tilde{I}_j(i_1)^3] \mathbb{E}[\tilde{I}_k(i_2)^3] \right. \right. \\ &\quad + 9\mathbb{E}[\tilde{I}_j(i_1)^2 \tilde{I}_k(i_1)^2] \mathbb{E}[\tilde{I}_j(i_2) \tilde{I}_k(i_2)] + 3\mathbb{E}[\tilde{I}_j(i_1)^3 \tilde{I}_k(i_1)] \mathbb{E}[\tilde{I}_k(i_2)^2] \Big\} \\ &\quad + 3\mathbb{E}[\tilde{I}_k(i_1)^3 \tilde{I}_j(i_1)] \mathbb{E}[\tilde{I}_j(i_2)^2] \\ &\quad + \sum_{i_1=1}^n \sum_{i_2 \neq i_1}^n \sum_{i_3 \neq i_1, i_2}^n \left\{ 9\mathbb{E}[\tilde{I}_j(i_1)^2] \mathbb{E}[\tilde{I}_j(i_2) \tilde{I}_k(i_2)] \mathbb{E}[\tilde{I}_k(i_3)^2] \right. \\ &\quad \left. \left. + 6\mathbb{E}[\tilde{I}_j(i_1) \tilde{I}_k(i_1)] \mathbb{E}[\tilde{I}_j(i_2) \tilde{I}_k(i_2)] \mathbb{E}[\tilde{I}_j(i_3) \tilde{I}_k(i_3)] \right\} \right\}. \end{aligned} \tag{21}$$

We now calculate the expectations in the above expression. We have that $\mathbb{E}[\tilde{I}_j(i_2)^2] = \text{Var}(I_j(i_2)) = p_j(1 - p_j)$. Also, by a routine calculation (or using a standard formula for the third central moment of the Bernoulli distribution), we have that $\mathbb{E}[\tilde{I}_j(i_1)^3] = p_j(1 - p_j)(1 - 2p_j)$. For the more complex expectations involving products of powers of $\tilde{I}_j(i_1)$ and $\tilde{I}_k(i_1)$, $j \neq k$, we use the fact that each trial leads to a unique classification. For $u, v \in \mathbb{N}$,

$$\begin{aligned} \mathbb{E}[\tilde{I}_j(i_1)^u \tilde{I}_k(i_1)^v] &= \mathbb{E}[(I_j(i_1) - p_j)^u (I_k(i_1) - p_k)^v] \\ &= -p_j^u (1 - p_k)^v \mathbb{P}(I_k(i_1) = 1) - p_k^v (1 - p_j)^u \mathbb{P}(I_j(i_1) = 1) \\ &\quad + p_j^u p_k^v \mathbb{P}(I_j(i_1) = I_k(i_1) = 0) \\ &= -p_j^u (1 - p_k)^v p_k - p_k^v (1 - p_j)^u p_j + p_j^u p_k^v (1 - p_j - p_k) \\ &= p_j p_k [-p_j^{u-1} (1 - p_k)^v - p_k^{v-1} (1 - p_j)^u + (1 - p_j - p_k) p_j^{u-1} p_k^{v-2}]. \end{aligned}$$

In the case $u = v = 1$, we have the simplification $\mathbb{E}[\tilde{I}_j(i_1) \tilde{I}_k(i_1)] = -p_j p_k$. Substituting these formulas for the expectations present in (21) now gives us

$$\begin{aligned} \mathbb{E}[S_j^3 S_k^3] &= \frac{1}{n^3(p_j p_k)^{3/2}} \left[n \cdot p_j p_k [-p_j^2 (1 - p_k)^3 - p_k^2 (1 - p_j)^3 + (1 - p_j - p_k)(p_j p_k)^2] \right. \\ &\quad + n(n - 1) \left\{ (p_j p_k (1 - p_j)(1 - p_k)(1 - 2p_j)(1 - 2p_k)) \right. \\ &\quad + 9 \left((p_j p_k)^2 [p_k (1 - p_j)^2 + p_j (1 - p_k)^2 + p_j + p_k - 1] \right) \\ &\quad + 3 \left(p_j p_k^2 (1 - p_k)(1 - 2p_k) [1 - p_j - p_k - p_j^2 (1 - p_k) - (1 - p_j)^3] \right) \\ &\quad \left. + 3 \left(p_j^2 p_k (1 - p_j)(1 - 2p_j) [1 - p_k - p_j - p_k^2 (1 - p_j) - (1 - p_k)^3] \right) \right\} \\ &\quad \left. + n(n - 1)(n - 2) \left\{ 9 \left(-(p_j p_k)^2 (1 - p_j)(1 - p_k) \right) + 6 \left(-(p_j p_k)^3 \right) \right\} \right]. \end{aligned}$$

Elementary calculations that make use of the facts that $p_j, p_k \in (0, 1)$ and that $0 \leq p_j + p_k \leq 1$ now yield the bound

$$\begin{aligned}
 |\mathbb{E}[S_j^3 S_k^3]| &\leq \frac{1}{n^3 (p_j p_k)^{3/2}} \left\{ np_j p_k + n^2 p_j p_k + 9n^2 (p_j p_k)^2 + 3n^2 p_j p_k^2 + 3n^2 p_j^2 p_k \right. \\
 &\quad \left. + 9n^3 (p_j p_k)^2 + 6n^3 (p_j p_k)^3 \right\} \\
 &= \frac{1}{n^2 \sqrt{p_j p_k}} + \frac{1}{4n \sqrt{p_j p_k}} + \frac{9\sqrt{p_j p_k}}{n} + \frac{3p_k^{3/2}}{n\sqrt{p_j}} + \frac{3p_j^{3/2}}{n\sqrt{p_k}} + \frac{9}{4}\sqrt{p_j p_k} + 6(p_j p_k)^{3/2} \\
 &= \frac{1}{n \cdot n \sqrt{p_j p_k}} + \frac{1}{4n \sqrt{p_j p_k}} + \frac{9p_j p_k}{n \sqrt{p_j p_k}} + \frac{3\sqrt{p_j p_k}^{3/2}}{np_j} + \frac{3p_j^{3/2} \sqrt{p_k}}{np_k} + \frac{9}{4}\sqrt{p_j p_k} \\
 &\quad + 6(p_j p_k) \cdot \sqrt{p_j p_k}. \tag{22}
 \end{aligned}$$

In obtaining this bound we did not attempt to optimise numerical constants, although in bounding the second and sixth terms we did take advantage of the simple inequality $(1 - p_j)(1 - p_k) \leq 1/4$ (maximum at $p_j = p_k = 1/2$). The final equality in (22) was given in anticipation of obtaining our final bound (20) for $|\mathbb{E}[S_j^3 S_k^3]|$. We now bound the terms in (22) using the following considerations. By assumption, $np_j \geq r$ for all $j = 1, \dots, r$, which also implies that $n \geq 4$, as $r \geq 2$. Moreover, for $j \neq k$, $p_j p_k \leq 1/4$ (maximised for $p_j = p_k = 1/2$) and $\sqrt{p_j p_k}^{3/2} \leq 3\sqrt{3}/16$ (maximised at $p_j = 1/4, p_k = 3/4$), with the same bound holding for $p_j^{3/2} \sqrt{p_k}$ by symmetry. With these considerations, we arrive at the bound

$$|\mathbb{E}[S_j^3 S_k^3]| \leq \frac{1}{4r} + \frac{1}{4r} + \frac{9}{4r} + 2 \cdot 3 \cdot \frac{3\sqrt{3}}{16r} + \frac{9}{4}\sqrt{p_j p_k} + \frac{6}{4}\sqrt{p_j p_k} < \frac{6}{r} + 4\sqrt{p_j p_k},$$

where in obtaining the second inequality we rounded the numerical constants up to the nearest integer. The proof of the lemma is complete. \square

The following lemma, which is proved in Appendix B, will be needed in the proof of Theorem 2. Lemma 5 below will be needed in the proof of Theorem 3. The proof of Lemma 5 is similar to that of Lemma 4 and is given in the Supplementary Information.

Lemma 4. *Let $a > 0$. Then,*

(i) *For $x \geq 0$,*

$$\left| 2x \log\left(\frac{x}{a}\right) - 2(x - a) - \frac{(x - a)^2}{a} + \frac{(x - a)^3}{3a^2} \right| \leq \frac{2(x - a)^4}{3a^3}. \tag{23}$$

(ii) *Suppose $\lambda \geq 3$. Then, for $x \geq 0$,*

$$\begin{aligned}
 &\left| \frac{x^{\lambda+1}}{a^\lambda} - a - (\lambda + 1)(x - a) - \frac{\lambda(\lambda + 1)}{2a}(x - a)^2 - \frac{(\lambda - 1)\lambda(\lambda + 1)}{6a^2}(x - a)^3 \right| \\
 &\leq \frac{(\lambda - 2)(\lambda - 1)\lambda(\lambda + 1)}{24} \left(1 + \left(\frac{x}{a}\right)^{\lambda-3} \right) \frac{(x - a)^4}{a^3}. \tag{24}
 \end{aligned}$$

(iii) Suppose $\lambda \in (-1, 3) \setminus \{0\}$. Then, for $x \geq 0$,

$$\left| \frac{x^{\lambda+1}}{a^\lambda} - a - (\lambda + 1)(x - a) - \frac{\lambda(\lambda + 1)}{2a}(x - a)^2 - \frac{(\lambda - 1)\lambda(\lambda + 1)}{6a^2}(x - a)^3 \right| \leq \frac{|(\lambda - 2)(\lambda - 1)\lambda|}{6} \frac{(x - a)^4}{a^3}. \tag{25}$$

Lemma 5. Let $a > 0$. Then,

(i) For $x \geq 0$,

$$\left| 2x \log\left(\frac{x}{a}\right) - 2(x - a) - \frac{(x - a)^2}{a} \right| \leq \frac{|x - a|^3}{a^2}. \tag{26}$$

(ii) Suppose $\lambda \geq 2$. Then, for $x \geq 0$,

$$\left| \frac{x^{\lambda+1}}{a^\lambda} - a - (\lambda + 1)(x - a) - \frac{\lambda(\lambda + 1)}{2a}(x - a)^2 \right| \leq \frac{(\lambda - 1)\lambda(\lambda + 1)}{6} \left(1 + \left(\frac{x}{a}\right)^{\lambda-2} \right) \frac{|x - a|^3}{a^2}. \tag{27}$$

(iii) Suppose $\lambda \in (-1, 2) \setminus \{0\}$. Then, for $x \geq 0$,

$$\left| \frac{x^{\lambda+1}}{a^\lambda} - a - (\lambda + 1)(x - a) - \frac{\lambda(\lambda + 1)}{2a}(x - a)^2 \right| \leq \frac{|(\lambda - 1)\lambda|}{2} \frac{|x - a|^3}{a^2}. \tag{28}$$

4. Proofs of main results

In this section we prove all the results stated in Section 2, except for Theorem 1, which is proved in Appendix A. We begin by introducing some notation and make some basic observations regarding the power divergence statistic T_λ .

For $j = 1, \dots, r$, let $S_j = (U_j - np_j) / \sqrt{np_j}$ denote the standardised cell counts, and let $S = (S_1, \dots, S_r)^\top$. Observe that $\sum_{j=1}^r U_j = n$ and $\sum_{j=1}^r \sqrt{p_j} S_j = 0$, and that $U_j \sim \text{Bin}(n, p_j)$, $j = 1, \dots, r$. With this notation, we may write the power divergence statistic T_λ , Pearson’s statistic χ^2 , and the likelihood ratio statistic L as

$$T_\lambda = \frac{2}{\lambda(\lambda + 1)} \left[\sum_{j=1}^r np_j \left(1 + \frac{S_j}{\sqrt{np_j}} \right)^{\lambda+1} - n \right], \quad \chi^2 = \sum_{j=1}^r S_j^2,$$

$$L = T_0 = 2 \sum_{j=1}^r (np_j + \sqrt{np_j} S_j) \log \left(1 + \frac{S_j}{\sqrt{np_j}} \right).$$

Proof of Theorem 2. For our purpose of deriving an order n^{-1} bound, it will be convenient to write the power divergence statistic T_λ in the form

$$T_\lambda = \sum_{j=1}^r S_j^2 + \frac{\lambda - 1}{3} \sum_{j=1}^r \frac{S_j^3}{\sqrt{np_j}} + R_\lambda(S),$$

where, for $\lambda \in (-1, \infty) \setminus \{0\}$,

$$R_\lambda(\mathbf{S}) = \frac{2}{\lambda(\lambda + 1)} \sum_{j=1}^r \left[np_j \left(1 + \frac{S_j}{\sqrt{np_j}} \right)^{\lambda+1} - np_j - (\lambda + 1)\sqrt{np_j}S_j - \frac{\lambda(\lambda + 1)}{2}S_j^2 - \frac{(\lambda - 1)\lambda(\lambda + 1)}{6\sqrt{np_j}}S_j^3 \right],$$

and, for $\lambda = 0$,

$$R_0(\mathbf{S}) = \sum_{j=1}^r \left[2(np_j + \sqrt{np_j}S_j) \log \left(1 + \frac{S_j}{\sqrt{np_j}} \right) - 2\sqrt{np_j}S_j - S_j^2 - \frac{S_j^3}{3\sqrt{np_j}} \right].$$

Here we used that $\sum_{j=1}^r p_j = 1$ and $\sum_{j=1}^r \sqrt{p_j}S_j = 0$.

Let us now bound the quantity of interest, $|\mathbb{E}[h(T_\lambda)] - \chi_{(r-1)}^2 h|$. By a first-order Taylor expansion and the triangle inequality we have that

$$\begin{aligned} |\mathbb{E}[h(T_\lambda)] - \chi_{(r-1)}^2 h| &= \left| \mathbb{E} \left[h \left(\sum_{j=1}^r S_j^2 + \frac{\lambda - 1}{3} \sum_{j=1}^r \frac{S_j^3}{\sqrt{np_j}} + R_\lambda(\mathbf{S}) \right) \right] - \chi_{(r-1)}^2 h \right| \\ &\leq \left| \mathbb{E} \left[h \left(\sum_{j=1}^r S_j^2 + \frac{\lambda - 1}{3} \sum_{j=1}^r \frac{S_j^3}{\sqrt{np_j}} \right) \right] - \chi_{(r-1)}^2 h \right| + R_1, \end{aligned}$$

where $R_1 = \|h'\| \mathbb{E}|R_\lambda(\mathbf{S})|$. Another Taylor expansion and application of the triangle inequality gives us the bound $|\mathbb{E}[h(T_\lambda)] - \chi_{(r-1)}^2 h| \leq R_1 + R_2 + R_3 + R_4$, where

$$\begin{aligned} R_2 &= |\mathbb{E}[h(\chi^2)] - \chi_{(r-1)}^2 h|, \\ R_3 &= \frac{|\lambda - 1|}{3} \left| \mathbb{E} \left[\sum_{j=1}^r \frac{S_j^3}{\sqrt{np_j}} h' \left(\sum_{k=1}^r S_k^2 \right) \right] \right|, \\ R_4 &= \frac{(\lambda - 1)^2}{18} \|h''\| \mathbb{E} \left[\left(\sum_{j=1}^r \frac{S_j^3}{\sqrt{np_j}} \right)^2 \right], \end{aligned}$$

and we recall that Pearson's statistic is given by $\chi^2 = \sum_{j=1}^r S_j^2$.

We can bound the remainder R_2 immediately using either (4) or (6). To bound R_3 , we recall another bound of [14] (see the bound for $|\mathbb{E}h_2(\mathbf{S})|$ given on p. 747): for $j = 1, \dots, r$,

$$\left| \mathbb{E} \left[S_j^3 h' \left(\sum_{k=1}^r S_k^2 \right) \right] \right| \leq \{2\|h'\| + 202\|h''\| + 819\|h^{(3)}\| + 100\,974\|h^{(4)}\|\} \sum_{k=1}^r \frac{1}{\sqrt{np_k}}.$$

Using this inequality, we obtain the bound

$$R_3 \leq \frac{|\lambda - 1|}{3n} \left(\sum_{j=1}^r \frac{1}{\sqrt{p_j}} \right)^2 \{2\|h'\| + 202\|h''\| + 819\|h^{(3)}\| + 100\,974\|h^{(4)}\|\}.$$

Let us now bound R_4 . Using the moment bounds (18) and (20) (our assumption that $np_j \geq r$ for all $j = 1, \dots, r$ allows us to apply this bound) gives

$$\begin{aligned} \mathbb{E} \left[\left(\sum_{j=1}^r \frac{S_j^3}{\sqrt{np_j}} \right)^2 \right] &= \sum_{j=1}^r \frac{\mathbb{E}[S_j^6]}{np_j} + \sum_{j=1}^r \sum_{k \neq j}^r \frac{\mathbb{E}[S_j^3 S_k^3]}{n \sqrt{p_j p_k}} \\ &\leq \sum_{j=1}^r \frac{28}{np_j} + \sum_{j=1}^r \sum_{k \neq j}^r \left\{ \frac{6}{nr \sqrt{p_j p_k}} + \frac{4}{n} \right\} \leq \frac{38}{nr} \left(\sum_{j=1}^r \frac{1}{\sqrt{p_j}} \right)^2. \end{aligned}$$

Therefore,

$$R_4 \leq \frac{19(\lambda - 1)^2}{9nr} \|h''\| \left(\sum_{j=1}^r \frac{1}{\sqrt{p_j}} \right)^2.$$

Lastly, we bound R_1 . We consider the cases $\lambda = 0$ (the likelihood ratio statistic), $\lambda \geq 3$, and $\lambda \in (-1, 3) \setminus \{0\}$ separately. Using that $S_j = (U_j - np_j) / \sqrt{np_j}$ and then applying inequality (23) of Lemma 4, we have that, for $\lambda = 0$,

$$\begin{aligned} R_1 &= \|h'\| \mathbb{E}|R_0(\mathbf{S})| \\ &= \|h'\| \mathbb{E} \left| \sum_{j=1}^r \left[2U_j \log \left(\frac{U_j}{np_j} \right) - 2(U_j - np_j) - \frac{(U_j - np_j)^2}{np_j} + \frac{(U_j - np_j)^3}{3(np_j)^2} \right] \right| \\ &\leq \frac{2\|h'\|}{3} \sum_{j=1}^r \frac{\mathbb{E}[(U_j - np_j)^4]}{(np_j)^3} \leq \frac{8\|h'\|}{3} \sum_{j=1}^r \frac{1}{np_j}, \end{aligned} \tag{29}$$

where we used that $\mathbb{E}[(U_j - np_j)^4] \leq 4(np_j)^2$ in the final step (see (17)).

Suppose now that $\lambda \geq 3$. Applying inequality (24) of Lemma 4, we have, for $\lambda \geq 3$,

$$\begin{aligned} R_1 &= \|h'\| \mathbb{E}|R_\lambda(\mathbf{S})| \\ &= \frac{2\|h'\|}{\lambda(\lambda + 1)} \mathbb{E} \left| \sum_{j=1}^r \left[\frac{U_j^{\lambda+1}}{(np_j)^\lambda} - np_j - (\lambda + 1)(U_j - np_j) - \frac{\lambda(\lambda + 1)(U_j - np_j)^2}{2 np_j} \right. \right. \\ &\quad \left. \left. - \frac{(\lambda - 1)\lambda(\lambda + 1)(U_j - np_j)^3}{6 (np_j)^2} \right] \right| \end{aligned} \tag{30}$$

$$\begin{aligned} &\leq \frac{(\lambda - 2)(\lambda - 1)\|h'\|}{12} \sum_{j=1}^r \mathbb{E} \left[\left(1 + \frac{U_j^{\lambda-3}}{(np_j)^{\lambda-3}} \right) \frac{(U_j - np_j)^4}{(np_j)^3} \right] \\ &\leq \frac{(\lambda - 2)(\lambda - 1)\|h'\|}{12} \sum_{j=1}^r \left\{ \frac{\mathbb{E}[(U_j - np_j)^4]}{(np_j)^3} \right. \\ &\quad \left. + \frac{1}{(np_j)^\lambda} (\mathbb{E}[(U_j - np_j)^6])^{2/3} (\mathbb{E}[U_j^{3\lambda-9}])^{1/3} \right\} \\ &\leq \frac{(\lambda - 2)(\lambda - 1)\|h'\|}{12} \sum_{j=1}^r \left\{ \frac{4}{np_j} + \frac{28^{2/3} \times (e^{9/4})^{1/3}}{np_j} \right\} \\ &\leq 2(\lambda - 2)(\lambda - 1)\|h'\| \sum_{j=1}^r \frac{1}{np_j}. \end{aligned} \tag{31}$$

Here we used Hölder’s inequality to obtain the second inequality; to get the third inequality we used the moment bounds (17), (18), and (19), respectively, $\mathbb{E}[(U_j - np_j)^4] \leq 4(np_j)^2$, $\mathbb{E}[(U_j - np_j)^6] \leq 28(np_j)^3$, and $\mathbb{E}[U_j^{3\lambda-9}] \leq e^{9/4}(np_j)^{3\lambda-9}$, where the latter bound is valid due to our assumption that $np_* \geq 2(\lambda - 3)^2$ for $\lambda \geq 3$.

Lastly, we consider the case $\lambda \in (-1, 3) \setminus \{0\}$. Applying inequality (25) of Lemma 4 to (30) and proceeding as before gives that, for $\lambda \in (-1, 3) \setminus \{0\}$,

$$R_1 \leq \frac{|\lambda - 2|(\lambda - 1)|\|h'\|}{6(\lambda + 1)} \sum_{j=1}^r \frac{\mathbb{E}[(U_j - np_j)^4]}{(np_j)^3} \leq \frac{2|\lambda - 2|(\lambda - 1)|\|h'\|}{3(\lambda + 1)} \sum_{j=1}^r \frac{1}{np_j}. \tag{32}$$

To obtain a universal bound on $|\mathbb{E}[h(T_\lambda)] - \chi_{(r-1)}^2 h|$ that is valid for all $\lambda > -1$, we observe that we can take the following upper bound for R_1 (valid for $\lambda \geq 3$ under the condition that $np_* \geq 2(\lambda - 3)^2$),

$$R_1 \leq \frac{|\lambda - 1|(\lambda - 2)(12\lambda + 13)|\|h'\|}{6(\lambda + 1)} \sum_{j=1}^r \frac{1}{np_j}, \tag{33}$$

which can be seen to be greater than each of the upper bounds (29), (31), and (32) that were obtained for the cases $\lambda = 0$, $\lambda \geq 3$, and $\lambda \in (-1, 3) \setminus \{0\}$, respectively.

Finally, we sum up our bound in (33) for R_1 and our bounds for R_2, R_3 , and R_4 . To obtain a compact final bound we use the inequality $(\sum_{j=1}^r p_j^{-1/2})^2 \leq r \sum_{j=1}^r p_j^{-1}$, which follows from the Cauchy–Schwarz inequality. Using (4) to bound R_2 gives us the bound in (10), while using (6) to bound R_2 yields (11). This completes the proof. \square

Remark 6. It was a fortunate accident that the term R_3 had previously been bounded in [14]. That this term is $O(n^{-1})$ is in some sense the key reason as to why the $O(n^{-1})$ rate is attained. Indeed, through our use of Taylor expansions we could guarantee that the remainder terms R_1 and R_4 would be $O(n^{-1})$, and $R_2 = |\mathbb{E}[h(\chi^2)] - \chi_{(r-1)}^2 h|$ had, of course, already been shown to be $O(n^{-1})$ by [14]. To give a self-contained account as to why the $O(n^{-1})$ rate is attained, we therefore briefly sketch why $R_3 = O(n^{-1})$.

Let $g(s) = \sum_{j=1}^r p_j^{-1/2} s_j^3 h'(\sum_{k=1}^r s_k^2)$. Observe that $g(-s) = -g(s)$. Now, let \mathbf{Z} be a centered r -dimensional multivariate normal random vector with covariance matrix equal to that of \mathbf{S} . Then, because $\mathbf{Z} \stackrel{d}{=} -\mathbf{Z}$, we have that $\mathbb{E}[g(\mathbf{Z})] = -\mathbb{E}[g(-\mathbf{Z})] = -\mathbb{E}[g(\mathbf{Z})]$, so that $\mathbb{E}[g(\mathbf{Z})] = 0$. Therefore,

$$R_3 = \frac{|\lambda - 1|}{3\sqrt{n}} |\mathbb{E}[g(\mathbf{S})]| = \frac{|\lambda - 1|}{3\sqrt{n}} |\mathbb{E}[g(\mathbf{S})] - \mathbb{E}[g(\mathbf{Z})]|.$$

The quantity $|\mathbb{E}[g(\mathbf{S})] - \mathbb{E}[g(\mathbf{Z})]|$ can then be bounded to order $O(n^{-1/2})$ by Stein’s method for multivariate normal approximation with polynomial growth rate test functions [13].

Proof of Theorem 3. The proof is similar to that of Theorem 2, but a little shorter and simpler. For our aim of obtaining an order $n^{-1/2}$ bound, we express T_λ in the form $T_\lambda = \sum_{j=1}^r S_j^2 + R_\lambda(\mathbf{S}) = \chi^2 + R_\lambda(\mathbf{S})$, where, for $\lambda \in (-1, \infty) \setminus \{0\}$,

$$R_\lambda(\mathbf{S}) = \frac{2}{\lambda(\lambda + 1)} \sum_{j=1}^r \left[np_j \left(1 + \frac{S_j}{\sqrt{np_j}} \right)^{\lambda+1} - np_j - (\lambda + 1)\sqrt{np_j} S_j - \frac{\lambda(\lambda + 1)}{2} S_j^2 \right]$$

and, for $\lambda = 0$,

$$R_0(S) = \sum_{j=1}^r \left[2(np_j + \sqrt{np_j}S_j) \log \left(1 + \frac{S_j}{\sqrt{np_j}} \right) - 2\sqrt{np_j}S_j - S_j^2 \right].$$

Now, by a first-order Taylor expansion and the triangle inequality we have that

$$|\mathbb{E}[h(T_\lambda)] - \chi_{(r-1)}^2 h| = |\mathbb{E}[h(\chi^2 + R_\lambda(S))] - \chi_{(r-1)}^2 h| \leq |\mathbb{E}[h(\chi^2)] - \chi_{(r-1)}^2 h| + R_1,$$

where $R_1 = \|h'\| \mathbb{E}|R_\lambda(S)|$.

The quantity $|\mathbb{E}[h(\chi^2)] - \chi_{(r-1)}^2 h|$ can be immediately bounded using either (5) or (7). To bound R_1 , we consider the cases $\lambda = 0$, $\lambda \geq 2$, and $\lambda \in (-1, 2) \setminus \{0\}$ separately. For $\lambda = 0$, using inequality (26) of Lemma 5 we obtain the bound

$$\begin{aligned} R_1 &= \|h'\| \mathbb{E} \left| \sum_{j=1}^r \left[2U_j \log \left(\frac{U_j}{np_j} \right) - 2(U_j - np_j) - \frac{(U_j - np_j)^2}{np_j} \right] \right| \\ &\leq \|h'\| \sum_{j=1}^r \frac{\mathbb{E}[|U_j - np_j|^3]}{(np_j)^2} \leq 3\|h'\| \sum_{j=1}^r \frac{1}{\sqrt{np_j}}, \end{aligned} \tag{34}$$

where we used inequality (16) in the final step.

For $\lambda \geq 2$ we use inequality (27) of Lemma 5 to get

$$\begin{aligned} R_1 &= \frac{2\|h'\|}{\lambda(\lambda + 1)} \mathbb{E} \left| \sum_{j=1}^r \left[\frac{U_j^{\lambda+1}}{(np_j)^\lambda} - np_j - (\lambda + 1)(U_j - np_j) - \frac{\lambda(\lambda + 1)}{2} \frac{(U_j - np_j)^2}{np_j} \right] \right| \\ &\leq \frac{(\lambda - 1)\|h'\|}{3} \sum_{j=1}^r \mathbb{E} \left[\left(1 + \frac{U_j^{\lambda-2}}{(np_j)^{\lambda-2}} \right) \frac{|U_j - np_j|^3}{(np_j)^2} \right] \\ &\leq \frac{(\lambda - 1)\|h'\|}{3} \sum_{j=1}^r \left\{ \frac{\mathbb{E}[|U_j - np_j|^3]}{(np_j)^2} + \frac{1}{(np_j)^\lambda} (\mathbb{E}[(U_j - np_j)^6])^{1/2} (\mathbb{E}[U_j^{2\lambda-4}])^{1/2} \right\} \\ &\leq \frac{(\lambda - 1)\|h'\|}{3} \sum_{j=1}^r \left\{ \frac{3}{\sqrt{np_j}} + \frac{28^{1/2} \times e^{1/2}}{\sqrt{np_j}} \right\} \leq 4(\lambda - 1)\|h'\| \sum_{j=1}^r \frac{1}{\sqrt{np_j}}. \end{aligned} \tag{35}$$

Here we used the Cauchy–Schwarz inequality to obtain the second inequality; to get the third inequality we used the moment bounds (16), (18), and (19), respectively, $\mathbb{E}[(U_j - np_j)^4] \leq 4(np_j)^2$, $\mathbb{E}[(U_j - np_j)^6] \leq 28(np_j)^3$, and $\mathbb{E}[U_j^{2\lambda-4}] \leq e(np_j)^{2\lambda-4}$, where the latter bound is valid due to our assumption that $np_* \geq 2(\lambda - 2)^2$ for $\lambda \geq 2$.

Lastly, we consider the case $\lambda \in (-1, 2) \setminus \{0\}$. Using inequality (28) of Lemma 5 on (30) and proceeding as before gives that, for $\lambda \in (-1, 2) \setminus \{0\}$,

$$R_1 \leq \frac{|\lambda - 1|\|h'\|}{\lambda + 1} \sum_{j=1}^r \frac{\mathbb{E}[|U_j - np_j|^3]}{(np_j)^2} \leq \frac{3|\lambda - 1|\|h'\|}{\lambda + 1} \sum_{j=1}^r \frac{1}{\sqrt{np_j}}. \tag{36}$$

To obtain a universal bound on $|\mathbb{E}[h(T_\lambda)] - \chi^2_{(r-1)}h|$ that is valid for all $\lambda > -1$, we observe that we can take the following upper bound for R_1 (valid for $\lambda \geq 2$ provided $np_* \geq 2(\lambda - 2)^2$),

$$R_1 \leq \frac{|\lambda - 1|(4\lambda + 7)|\|h'\|}{\lambda + 1} \sum_{j=1}^r \frac{1}{\sqrt{np_j}}, \tag{37}$$

which can be seen to be greater than each of the upper bounds (34), (35), and (36) that were obtained for the cases $\lambda = 0$, $\lambda \geq 2$, and $\lambda \in (-1, 2) \setminus \{0\}$, respectively.

Summing up our bound (37) for R_1 and either the bound (5) or the bound (7) for $|\mathbb{E}[h(\chi^2)] - \chi^2_{(r-1)}h|$ now yields the desired bounds (12) and (13), respectively. \square

Proof of Corollary 1. Let $\alpha > 0$ and, for fixed $z > 0$, define

$$h_\alpha(x) = \begin{cases} 1, & \text{if } x \leq z, \\ 1 - 2(x - z)^2/\alpha^2, & \text{if } z < x \leq z + \alpha/2, \\ 2(x - (z + \alpha))^2/\alpha^2, & \text{if } z + \alpha/2 < x \leq z + \alpha, \\ 0, & \text{if } x \geq z + \alpha. \end{cases}$$

Then h'_α is Lipschitz with $\|h_\alpha\| = 1$, $\|h'_\alpha\| = 2/\alpha$, and $\|h''_\alpha\| = 4/\alpha^2$. Let $Y_{r-1} \sim \chi^2_{(r-1)}$. Then, using (12), together with the basic inequality $\sum_{j=1}^r p_j^{-1/2} \leq r/\sqrt{p_*}$, gives

$$\begin{aligned} & \mathbb{P}(T_\lambda \leq z) - \mathbb{P}(Y_{r-1} \leq z) \\ & \leq \mathbb{E}[h_\alpha(T_\lambda)] - \mathbb{E}[h_\alpha(Y_{r-1})] + \mathbb{E}[h_\alpha(Y_{r-1})] - \mathbb{P}(Y_{r-1} \leq z) \\ & \leq \frac{1}{\sqrt{np_*}} \left\{ 72\|h_\alpha\| + \left(552 + \frac{|\lambda - 1|(4\lambda + 7)r}{\lambda + 1} \right) \|h'_\alpha\| + 1008\|h''_\alpha\| \right\} \\ & \quad + \mathbb{P}(z \leq Y_{r-1} \leq z + \alpha) \\ & = \frac{1}{\sqrt{np_*}} \left\{ 72 + \frac{1104}{\alpha} + \frac{|\lambda - 1|(4\lambda + 7)r}{(\lambda + 1)\alpha} + \frac{4032}{\alpha^2} \right\} + \mathbb{P}(z \leq Y_{r-1} \leq z + \alpha). \end{aligned} \tag{38}$$

It was shown in [14, p.754] that

$$\mathbb{P}(z \leq Y_{r-1} \leq z + \alpha) \leq \begin{cases} \sqrt{2\alpha/\pi}, & \text{if } r = 2, \\ \alpha/2, & \text{if } r = 3, \\ \frac{\alpha}{2\sqrt{\pi(r-3)}}, & \text{if } r \geq 4. \end{cases} \tag{39}$$

Upper bounds for the cases $r = 2$, $r = 3$, and $r \geq 4$ follow on substituting inequality (39) into (38) and selecting a suitable α . We choose $\alpha = 52.75(np_*)^{-1/5}$ for $r = 2$; we take $\alpha = 25.27(np_*)^{-1/6}$ when $r = 3$; and $\alpha = 30.58(r - 3)^{1/6}(np_*)^{-1/6}$ for $r \geq 4$. A lower bound can be obtained similarly, which is the negative of the upper bound. The proof is now complete. \square

Appendix A. Stein’s method for chi-square approximation and proof of Theorem 1

The first detailed study of Stein’s method for chi-square approximation was given in [21]. For further details on Stein’s method for chi-square approximation we refer the reader to

[9, 14, 24]. At the heart of Stein’s method for chi-square approximation is the following so-called *Stein equation* for the $\chi_{(p)}^2$ distribution (see [8]),

$$xf''(x) + \frac{1}{2}(p - x)f'(x) = h(x) - \chi_{(p)}^2 h, \tag{40}$$

where h is a real-valued test function and we recall that $\chi_{(d)}^2 h$ denotes the quantity $\mathbb{E}[h(Y_p)]$ for $Y_p \sim \chi_{(p)}^2$. It is straightforward to verify that

$$f'(x) = \frac{1}{x\rho(x)} \int_0^x (h(t) - \chi_{(p)}^2 h)\rho(t) dt, \tag{41}$$

where $\rho(x)$ denotes the $\chi_{(p)}^2$ density, solves the Stein equation (40) (see [35, Lemma 1, p. 59]).

Suppose we wish to obtain error bounds for the approximation of the distribution of a random variable of interest W and a $\chi_{(p)}^2$ distribution. The Stein equation (40) allows us to obtain bounds on the quantity of interest $|\mathbb{E}[h(W)] - \chi_{(p)}^2 h|$ by the following transfer principle: evaluate both sides of (40) at W and take expectations to obtain

$$|\mathbb{E}[h(W)] - \chi_{(p)}^2 h| = \mathbb{E}\left[Wf''(W) + \frac{1}{2}(p - W)f'(W)\right], \tag{42}$$

where f is the solution (41). Thus, the chi-square approximation problem is reduced to bounding the right-hand side of (42). For this procedure to be effective, one requires suitable estimates for the solution of the Stein equation together with certain lower-order derivatives of the solution. We now record some bounds for solution (41) that will be needed in the proof of Theorem 1.

We first state a bound from [21]. For $h \in C_b^{k,k}(\mathbb{R}^+)$,

$$\|f^{(k)}\| \leq \frac{2\|h^{(k)}\|}{k}, \quad k \geq 1. \tag{43}$$

The following bound from [12] improved a bound from [27]. For $h \in C_b^{k-1,k-1}(\mathbb{R}^+)$,

$$\|f^{(k)}\| \leq \left\{ \frac{\sqrt{2}(\sqrt{2\pi} + e^{-1})}{\sqrt{p + 2k - 2}} + \frac{4}{p + 2k - 2} \right\} \|h^{(k-1)}\|, \quad k \geq 1, \tag{44}$$

where $h^{(0)} \equiv h$. The conditions on the test function h for the bounds (43) and (44) are the same (but presented in a simpler manner) as those used in [14], in which it was noted that the bounds are valid under these conditions which are weaker than those presented in [21] and [12]. From (44), we deduce (using that $p \geq 1$ and $k \geq 2$) the simplified bounds

$$\|f^{(k)}\| \leq \frac{6.375\|h^{(k-1)}\|}{\sqrt{p + 1}}, \quad k \geq 2, \tag{45}$$

and

$$\|f^{(k)}\| \leq \left\{ \frac{\sqrt{2}(\sqrt{2\pi} + e^{-1})}{\sqrt{2k - 1}} + \frac{4}{2k - 1} \right\} \|h^{(k-1)}\|, \quad k \geq 2. \tag{46}$$

Finally, we record a bound from [14]. For $h \in C_b^{k-2,k-1}(\mathbb{R}^+)$,

$$\|f^{(k)}\| \leq \frac{4}{p + 2} (3\|h^{(k-1)}\| + 2\|h^{(k-2)}\|), \quad k \geq 2. \tag{47}$$

Proof of Theorem 1. In the proof of the bounds (4) and (5), [14] obtained the intermediate bounds

$$|\mathbb{E}[h(\chi^2)] - \chi_{(r-1)}^2 h| \leq \frac{1}{n} \{19\|f''\| + 309\|f^{(3)}\| + 1089\|f^{(4)}\| + 1997\|f^{(5)}\| + 100\,974\|f^{(6)}\|\} \left(\sum_{j=1}^r \frac{1}{\sqrt{p_j}}\right)^2 \tag{48}$$

and

$$|\mathbb{E}[h(\chi^2)] - \chi_{(r-1)}^2 h| \leq \frac{1}{\sqrt{n}} \{18\|f''\| + 84\|f^{(3)}\|\} \sum_{j=1}^r \frac{1}{\sqrt{p_j}}, \tag{49}$$

where f is the solution (41) of the $\chi_{(r-1)}^2$ Stein equation.

We note that bounding the derivatives of the solution f of the $\chi_{(r-1)}^2$ Stein equation in (48) and (49) using inequality (47) then yields the bounds (4) and (5), respectively. The bounds (6) and (7) of Theorem 1 are obtained by instead using inequality (45) to bound the derivatives of f in the bounds (4) and (5), respectively. To get the bound (8) of Theorem 1, we use the inequality (43) to bound $\|f''\|, \dots, \|f^{(5)}\|$ and (46) to bound $\|f^{(6)}\|$ in (48). Finally, to obtain the bound (9) we use (43) to bound $\|f''\|$ and (46) to bound $\|f^{(3)}\|$ in (49). \square

Appendix B. Proof of Lemma 4

Proof of Lemma 4. (i) Without loss of generality, we let $a = 1$; the general $a > 0$ case follows by rescaling. We therefore need to prove that, for $x \geq 0$,

$$|f(x)| \leq \frac{2}{3}(x - 1)^4, \tag{50}$$

where $f(x) := 2x \log(x) - 2(x - 1) - (x - 1)^2 + \frac{1}{3}(x - 1)^3$. It is readily checked that inequality (50) holds for $x = 0$ and $x = 2$. For $0 < x < 2$ (i.e. $|x - 1| < 1$), we can use a Taylor expansion to obtain the bound

$$|f(x)| = 2(x - 1)^4 \left| \sum_{k=0}^{\infty} \frac{(-1)^k (x - 1)^k}{(k + 3)(k + 4)} \right| \leq 2(x - 1)^4 \sum_{k=0}^{\infty} \frac{1}{(k + 3)(k + 4)} = \frac{2}{3}(x - 1)^4,$$

so inequality (50) is satisfied for $0 < x < 2$. Now, suppose $x > 2$. We have that $f'(x) = 2 \log(x) - 2(x - 1) + (x - 1)^2$ and $\frac{d}{dx}(2(x - 1)^4/3) = 8(x - 1)^3/3$. By the elementary inequality $\log(u) \leq u - 1$ for $u \geq 1$, we get that

$$\begin{aligned} |f'(x)| &= |2 \log(x) - 2(x - 1) + (x - 1)^2| \\ &= 2 \log(x) - 2(x - 1) + (x - 1)^2 \leq (x - 1)^2 \leq \frac{8}{3}(x - 1)^3, \end{aligned}$$

where the final inequality holds because $x > 2$. Therefore, for $x > 2$, $2(x - 1)^4/3$ grows faster than $|f(x)|$. Since $|f(2)| < 2(2 - 1)^4/3 = 2/3$, it follows that inequality (50) holds for all $x > 2$. We have now shown that (50) is satisfied for all $x \geq 0$, as required.

(ii) Suppose $\lambda \geq 3$. Again, without loss of generality, we may set $a = 1$. We therefore need to prove that, for $x \geq 0$,

$$|g_\lambda(x)| \leq \frac{(\lambda - 2)(\lambda - 1)\lambda(\lambda + 1)}{24} (1 + x^{\lambda-3})(x - 1)^4, \tag{51}$$

where

$$g_\lambda(x) := x^{\lambda+1} - 1 - (\lambda + 1)(x - 1) - \frac{\lambda(\lambda + 1)}{2}(x - 1)^2 - \frac{(\lambda - 1)\lambda(\lambda + 1)}{6}(x - 1)^3. \tag{52}$$

By a Taylor expansion of $x^{\lambda+1}$ about $x = 1$ we have that

$$g_\lambda(x) = \frac{(\lambda - 2)(\lambda - 1)\lambda(\lambda + 1)}{24}\xi^{\lambda-3}(x - 1)^4, \tag{53}$$

where $\xi > 0$ is between 1 and x . Now, as ξ is between 1 and x and because $\lambda \geq 3$, we have that $\xi^{\lambda-3} \leq (\max\{1, x\})^{\lambda-3} \leq 1 + x^{\lambda-3}$, and applying this inequality to (53) gives us (51), as required.

(iii) Suppose now that $\lambda \in (-1, 3) \setminus \{0\}$. Without loss of generality we set $a = 1$, and it therefore suffices to prove that, for $x \geq 0$,

$$|g_\lambda(x)| \leq \frac{|(\lambda - 2)(\lambda - 1)\lambda|}{6}(x - 1)^4. \tag{54}$$

We shall verify inequality (54) by treating the cases $0 < x \leq 2$ and $x \geq 2$ separately (it is readily checked that the inequality holds at $x = 0$). For $0 < x < 2$ (i.e. $|x - 1| < 1$) we can use a Taylor expansion to write $g_\lambda(x) = (x - 1)^4 G_\lambda(x)$, where

$$G_\lambda(x) = \sum_{k=0}^{\infty} \binom{\lambda + 1}{k + 4} (x - 1)^k,$$

and the generalised binomial coefficient is given by $\binom{a}{j} = [a(a - 1)(a - 2) \cdots (a - j + 1)]/j!$ for $a > 0$ and $j \in \mathbb{N}$. We now observe that, since $\lambda < 3$, the generalised binomial coefficients $\binom{\lambda+1}{k+4}$ are either positive for all even $k \geq 0$ and negative for all odd $k \geq 1$, or are negative for all even $k \geq 0$ and positive for all odd $k \geq 1$ (or, exceptionally, always equal to zero if $\lambda \in \{1, 2\}$, which is a trivial case in which $g_\lambda(x) = 0$ for all $x \geq 0$). Hence, for $0 < x < 2$, $G_\lambda(x)$ is bounded above by $|G_\lambda(0)|$, and a short calculation using the expression in (52) (note that $G_\lambda(x) = g_\lambda(x)/(x - 1)^4$) shows that $G_\lambda(0) = |(\lambda - 2)(\lambda - 1)\lambda|/6$. Thus, for $0 \leq x < 2$, we have the bound

$$|g_\lambda(x)| \leq \frac{|(\lambda - 2)(\lambda - 1)\lambda|}{6}(x - 1)^4.$$

Suppose now that $x \geq 2$. Recall from (53) that

$$g_\lambda(x) = \frac{(\lambda - 2)(\lambda - 1)\lambda(\lambda + 1)}{24}\xi^{\lambda-3}(x - 1)^4,$$

where $\xi > 0$ is between 1 and x . In fact, because we are considering the case $x \geq 2$, we know that $\xi > 1$. Therefore, since $\lambda < 3$, we have that $\xi^{\lambda-3} < 1$. Therefore, for $x \geq 2$,

$$|g_\lambda(x)| = \frac{|(\lambda - 2)(\lambda - 1)\lambda(\lambda + 1)|}{24}(x - 1)^4 \leq \frac{|(\lambda - 2)(\lambda - 1)\lambda|}{6}(x - 1)^4,$$

where the second inequality follows because $\lambda \in (-1, 3) \setminus \{0\}$. We have thus proved inequality (54), which completes the proof of the lemma. □

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Supplementary material

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