The asymptotic minimax risk for the estimation of constrained binomial and multinomial probabilities

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Abstract

In this paper we present a direct and simple approach to obtain bounds on the asymptotic minimax risk for the estimation of constrained binomial and multinomial proportions. Quadratic, normalized quadratic and entropy loss are considered and it is demonstrated that in all cases linear estimators are asymptotically minimax optimal. For the quadratic loss function the asymptotic minimax risk does not change unless a neighborhood of the point 1/2 is excluded by the restrictions on the parameter space. For the two other loss functions the asymptotic behavior of the minimax risk is not changed by such additional knowledge about the location of the unknown probability. The results are also extended to the problem of minimax estimation of a vector of constrained multinomial probabilities.

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1 Introduction

We consider the problem of estimating the unknown parameter θ of a binomial proportion

$$P_\theta(X = k) = B_{n,k}(\theta) := \binom{n}{k}\theta^k(1-\theta)^{n-k}, \quad 0 \le k \le n \tag{1.1}$$

where $0 \le \theta \le 1$. In many statistical problems the experimenter has definite prior information regarding the value of θ, often given in the form of bounds $0 \le a < b \le 1$ such that $\theta \in [a, b]$.

A commonly used approach to incorporate information of this type in the construction of an estimator is the minimax concept. A minimax estimate minimizes the maximal risk over the bounded parameter space $[a, b]$.

Usually neither the determination of a minimax estimate nor the calculation of the minimax risk (i.e. the risk of the minimax estimate) is a straightforward problem. For the problem of minimax estimation of the parameter of the binomial distribution over the bounded parameter space $[a, b] \subset [0, 1]$ Berry (1989) found minimax estimates for small values of n and squared error loss and a symmetric parameter space, i.e. $a = 1-b$. Recently Marchand and MacGibbon (2000) determined minimax estimators for the parameter space $[0, b]$ and quadratic and normalized quadratic loss, provided that the parameter b is smaller than a certain bound, say $b^*(n)$, which converges to 0 with increasing sample sizes. These authors also determined the linear minimax rules and corresponding risks for any bounded parameter space $[a, b]$; see also Lehn and Rummel (1987) for some related results on Gamma-minimax estimation of a binomial probability with restricted parameter space and Charras and van Eeden (1991) for some admissibility results in this context.

It is the purpose of the present paper to provide more information about this minimax estimation problem from an asymptotic point of view. We present a simple and direct approach to derive the asymptotic minimax risk for the estimation of a binomial probability, which is known to be in an interval $[a, b]$. We consider quadratic, normalized quadratic, and also the entropy loss. The asymptotic minimax risks for the these loss functions are determined for any interval $[a, b]$. If the point $1/2$ is *not contained* in the interval $[a, b]$, the asymptotic minimax risk with respect to the quadratic loss differs for the constrained and unconstrained case, while there are no asymptotic improvements if $\frac{1}{2} \in [a, b]$ or if the normalized quadratic or entropy loss function are chosen for the comparison of estimators. Some heuristical explanation of these phenomena is given in Remark 3.6. Our results also show that the linear minimax rules by Marchand and MacGibbon (2000) are asymptotically minimax optimal. The results are also extended to the situation, where the probability of success is known to be located in a more general set $\Theta \subset [0, 1]$ and to the problem of minimax estimation of a vector of constrained multinomial probabilities. The last-named problem has found much less attention in the literature. For some results regarding minimax estimation without restrictions on the vector of parameters we refer to the work of Steinhaus (1957), Trybula (1958, 1986), Olkin and Sobel (1977), Wilczynski (1985), He (1990) and Braess, Forster, Sauer, and Simon (2002) among many others.

The remaining part of this paper is organized as follows. Section 2 contains the necessary notation. The main results and some parts of the proofs for the binomial distribution are given in Section 3 while some more technical arguments are deferred to an appendix. Although the multinomial distribution contains the binomial as a special case, the latter case is treated separately in Section 4, mainly because we think that this organization facilitates the general reading of the paper.

2 Notation and point of departure

Consider the problem of estimating the parameter θ of the binomial distribution (1.1) and let

$$L : [0,1] \times [0,1] \to \mathbb{R}$$

denote a convex loss function. It is well known [see e.g. Ferguson (1967)] that for convex loss functions it is sufficient to consider nonrandomized rules of the form

$$\delta : \{0,1,2,\dots,n\} \to [0,1] \tag{2.1}$$

for the estimation of the probability θ. The quality of such an estimator is measured by the expected risk

$$R(\delta,\theta) := E_\theta[L(\theta,\delta(X))] = \sum_{k=0}^{n} B_{n,k}(\theta) L(\delta_k,\theta)\,, \tag{2.2}$$

where $B_{n,k}(\theta) := \binom{n}{k}\theta^(1-\theta)^{n-k}$ and we use the notation $\delta_k = \delta(k)$ for the sake of simplicity ($k = 0,\dots,n$). An estimator δ^* is called minimax with respect to the loss function L if

$$\sup_{a\le\theta\le b} R(\delta^*,\theta) = \inf_{\delta} \sup_{a\le\theta\le b} R(\delta,\theta),$$

where the infimum is taken over the class of all nonrandomized estimators. In this paper we consider the *quadratic loss function*

$$L_{qu}(q,p) := (p-q)^2, \tag{2.3}$$

the *normalized* or *standardized quadratic loss function*

$$L_{sq}(q,p) := \frac{(p-q)^2}{p(1-p)}\,, \tag{2.4}$$

and the *entropy loss function*

$$L_{KL}(q,p) := p\log\frac{p}{q} + (1-p)\log\frac{1-p}{1-q} \tag{2.5}$$

that is also called *Kullback–Leibler distance*. The loss functions (2.3) and (2.4) have been studied by Marchand and McGibbon (2000) in the same context while the entropy loss L_{KL} has been used for minimax estimation with an unconstrained parameter space by Cover (1972) and Wieczorkowski and Zieliński (1992), who obtained some numerical results. Braess and Sauer (2003) established sharp asymptotic bounds for the minimax risk with respect to this loss function if $[a,b] = [0,1]$.

In the unconstrained case the minimax rules for the loss functions (2.3), (2.4) are well known and given by the "add-β-rules"

$$\delta_k^\beta := \frac{k+\beta}{n+2\beta}, \quad k = 0,\dots,n, \tag{2.6}$$

where $\beta = \frac{1}{2}\sqrt{n}$ and $\beta = 0$, respectively; see Lehmann (1983). The phrase *add-β-rule* is adopted from learning theory [see Cover (1972), Krichevskiy (1998)], where minimax rules with respect to entropy loss are used to obtain optimal codings. In particular, add-β-rules are linear and have the symmetry property

$$\delta^\beta(k) + \delta^\beta(n-k) = 1. \tag{2.7}$$

The corresponding minimax risks are given by

$$\inf_\delta \sup_{\theta\in[0,1]} R_{qu}(\delta,\theta) = \frac{n}{4(n+\sqrt{n})^2}\,, \tag{2.8}$$

$$\inf_\delta \sup_{\theta\in[0,1]} R_{sq}(\delta,\theta) = \frac{1}{n}\,, \tag{2.9}$$

and

$$\inf_\delta \sup_{\theta\in[0,1]} R_{KL}(\delta,\theta) = \frac{1}{2n}(1+o(1)), \tag{2.10}$$

respectively. The asymptotic minimax estimate for the entropy loss is achieved by the combination of three add-β-rules, i.e.

$$\delta_k^{KL} = \begin{cases} \frac{1/2}{n+5/4} & k=0, \\ \frac{2}{n+7/4} & k=1, \\ \frac{k+3/4}{n+3/2} & k=2,\ldots,n-2, \\ \frac{n-1/4}{n+7/4} & k=n-1, \\ \frac{n+3/4}{n+5/4} & k=n; \end{cases} \tag{2.11}$$

see Braess and Sauer (2003).

3 Constrained minimax estimation of binomial probabilities

Our first result shows that the minimax rules remain asymptotically optimal if the parameter space is restricted to an interval $[a,b]$, which contains the point $1/2$.

Theorem 3.1 *Assume that $0 \le a < 1/2 < b \le 1$, then we have for $n\to\infty$*

$$\begin{aligned}
\inf_\delta \sup_{\theta\in[a.b]} R_{qu}(\delta,\theta) &= \frac{n}{4(n+\sqrt{n})^2}(1+O(n^{-1})) \;=\; \frac{1}{4n}(1+O(n^{-1/2})), \\
\inf_\delta \sup_{\theta\in[a,b]} R_{sq}(\delta,\theta) &= \frac{1}{n}(1+O(n^{-1/2})), \\
\inf_\delta \sup_{\theta\in[a,b]} R_{KL}(\delta,\theta) &= \frac{1}{2n}(1+o(1)).
\end{aligned}$$

Proof. The upper bounds are immediate from (2.8)–(2.10) because the maximal risk with respect to the restricted parameter space $[a, b] \subset [0, 1]$ is always smaller than the original one. The essential step is the proof of the lower bound for the risk with respect to the quadratic loss function.

We recall that the add-β-rule (2.6) with $\beta = \frac{1}{2}\sqrt{n}$ is the minimax estimate on the unrestricted interval; see Lehmann (1983), and it yields a constant risk function,

$$R_{qu}(\delta^{\frac{1}{2}\sqrt{n}}, \theta) = \frac{n}{4(n+\sqrt{n})^2}. \tag{3.1}$$

Now let $w_m(t) := c_m t^m (1-t)^m$ denote the beta-prior, where $m = \frac{1}{2}\sqrt{n} - 1$ and c_m is a normalizing constant such that w_m integrates to 1. Since we are concerned with lower bounds here, the normalization may refer to the integral over the (larger) interval $[0, 1]$. The rule $\delta^{\frac{1}{2}\sqrt{n}}$ is the Bayes estimate for quadratic loss on the unrestricted parameter space with respect to the prior w_m, i.e. we have for any estimate $\delta : \{0, 1, \ldots, n\} \to [a, b]$:

$$\int_0^1 R_{qu}(\delta, t) w_m(t) dt \geq \int_0^1 R_{qu}(\delta^{\frac{1}{2}\sqrt{n}}, t) w_m(t) dt = \frac{n}{4(n+\sqrt{n})^2}. \tag{3.2}$$

Next, note that for any estimate δ:

$$R_{qu}(\delta, \theta) \leq 1 \quad \text{for all } \theta \in [a, b]. \tag{3.3}$$

Therefore we obtain from (3.2) and (3.3) for any estimate $\delta : \{0, 1, \ldots, n\} \to [a, b]$:

$$\begin{aligned}
\sup_{\theta \in [a,b]} R_{qu}(\delta, \theta) &\geq \int_a^b R_{qu}(\delta, t) w_m(t) dt \\
&= \int_0^1 R_{qu}(\delta, t) w_m(t) dt - \Big(\int_0^a + \int_b^1\Big) R_{qu}(\delta, t) w_m(t) dt \\
&\geq \int_0^1 R_{qu}(\delta^{\frac{1}{2}\sqrt{n}}, t) w_m(t) dt - \Big(\int_0^a + \int_b^1\Big) w_m(t) dt. \qquad (3.4)
\end{aligned}$$

Now we use Lemma A.1 with $\alpha := 1/2$ and $s := \sqrt{n} - 2$ for estimating the integral over the interval $[0, a]$. The integral at the right boundary can be treated in the same way. Noting that $\int_0^1 w_m dt = 1$ we obtain for sufficiently large n the lower bound

$$\sup_{\theta \in [a,b]} R_{qu}(\delta, \theta) \geq \frac{n}{4(n+\sqrt{n})^2} - 2\frac{1}{n^2}\,, \tag{3.5}$$

which proves the assertion of Theorem 3.1 for the quadratic loss function.

The second part of the theorem regarding the normalized quadratic loss is now a simple consequence. From $\theta(1-\theta) \leq \frac{1}{4}$ it follows that

$$L_{sq}(\delta, \theta) \geq 4 L_{qu}(\delta, \theta) \tag{3.6}$$

holds for all arguments. Thus we have for any estimate $\delta : \{0,\ldots,k\} \to [0,1]$ and sufficiently large n:

$$\sup_{\theta\in[a,b]} R_{sq}(\delta,\theta) \geq 4 \sup_{\theta\in[a,b]} R_{qu}(\delta,\theta) \geq \frac{n}{(n+\sqrt{n})^2} + O\Big(\frac{1}{n^2}\Big) = \frac{1}{n}(1+O(n^{-1/2})).$$

An alternative proof which also covers the case $\frac{1}{2} \notin [a,b]$ and which is more direct will be provided in connection with Theorem 3.2.

For the remaining lower bound regarding the entropy loss function we also use a comparison and observe that

$$L_{KL}(q,q) = \frac{\partial}{\partial p} L_{KL}(q,p)\Big|_{p=q} = 0, \qquad \frac{\partial^2}{\partial p^2} L_{KL}(q,p) = \frac{1}{p(1-p)}.$$

Hence,

(3.7)
$$L_{KL}(q,p) \geq 2L_{qu}(q,p) := 2(p-q)^2.$$

From the result for the quadratic loss function we obtain as above

$$\inf_\delta \sup_{\theta\in[a,b]} R_{KL}(\delta,\theta) \;\geq\; 2\inf_\delta \sup_{\theta\in[a,b]} R_{qu}(\delta,\theta) \;=\; \frac{n}{2(n+\sqrt{n})^2}(1+O(n^{-1})) \;=\; \frac{1}{2n}(1+o(1)).$$

□

In the following we will investigate the situation where the point $1/2$ is not contained in the interval $[a,b]$. For the normalized quadratic and the entropy loss the asymptotic minimax risks remain unchanged, while there are differences for the quadratic loss function (2.3).

In the proof of Theorem 3.1 we used a prior distribution that is least favorable for the quadratic loss *and for finite* n. Therefore, we got the risk for the quadratic loss with a deviation of $O(n^{-1})$ as $n \to \infty$. In all other cases, the prior for the constrained domain differs from the prior for the full interval, and the deviation from the limit is only of order $O(n^{-1/2})$ or even $o(1)$. In this context we observe another feature. In many calculations of a minimax risk a prior is chosen such that the resulting risk function is a constant or nearly constant function of θ. This will be different in the analysis of restricted parameter spaces which do not contain the point $1/2$.

Theorem 3.2 *If* $0 \leq a < b \leq 1/2$, *then*

(3.8)
$$\inf_\delta \sup_{\theta\in[a,b]} R_{qu}(\delta,\theta) \;=\; \frac{b(1-b)}{n}(1+o(1)),$$

(3.9)
$$\inf_\delta \sup_{\theta\in[a,b]} R_{sq}(\delta,\theta) \;=\; \frac{1}{n}(1+O(n^{-1/2}))).$$

Proof. This time we start with the analysis of the normalized quadratic loss.

The upper bound in (3.9) is obvious from (2.9) again. The proof of the lower bound proceeds in the spirit of the proof of Theorem 3.1, but requires the use of a non symmetric beta-prior

(3.10)
$$w_{m,\ell}(t) := c_{m,\ell}\, t^m (1-t)^\ell$$

(here $c_{m,\ell}$ is again a normalizing constant), which makes the arguments more technical. The parameters m and ℓ will be fixed later such that the mode of the density $w_{m,\ell}$ is an interior point of the interval $[a,b]$ under consideration. The corresponding Bayes estimate (with respect to the normalized quadratic loss) is known to be

$$\delta^{m,\ell}(k) = \delta_k^{m,\ell} = \frac{k+m}{n+m+\ell}; \tag{3.11}$$

[see Lehmann (1983)]. We note that for $m \neq \ell$ this estimator does not possess the symmetry property (2.7). Sums of the Bernstein polynomials (1.1) with quadratic polynomials are easily treated [see e.g. Lorentz (1952)], and a straightforward calculation gives for the associated risk function

$$R_{sq}(\delta^{m,\ell},\theta) = \frac{1}{\theta(1-\theta)} \frac{1}{(n+m+\ell)^2} \{[(m+\ell)\theta - m]^2 + n\theta(1-\theta)\}.$$

We now fix $(m+\ell)^2 = n$, denote any corresponding estimate by δ^*, and obtain

$$R_{sq}(\delta^*,\theta) = \frac{1}{\theta(1-\theta)} \frac{1}{(n+\sqrt{n})^2}[m^2 + (n - 2m\sqrt{n})\theta]. \tag{3.12}$$

The corresponding Bayes risk is

$$\begin{aligned} \int_0^1 R_{sq}(\delta^*,t) w_{m,\ell}(t)dt &= \frac{1}{(n+\sqrt{n})^2}[\frac{m}{\ell}(n+\sqrt{n}) + \frac{\sqrt{n}+1}{\ell}(n-2m\sqrt{n})] \\ &= \frac{1}{n+\sqrt{n}}\ , \end{aligned} \tag{3.13}$$

where we used the condition $(m+\ell)^2 = n$ and the representations

$$\begin{aligned} \frac{c_{m,\ell}}{c_{m-1,\ell-1}} &= \frac{\int t^{m-1}(1-t)^{\ell-1}dt}{\int t^m(1-t)^\ell dt} = \frac{(m+\ell)(m+\ell+1)}{m\ell} = \frac{n+\sqrt{n}}{m\ell}, \\ \frac{c_{m,\ell}}{c_{m,\ell-1}} &= \frac{\int t^m(1-t)^{\ell-1}dt}{\int t^m(1-t)^\ell dt} = \frac{m+\ell+1}{\ell} = \frac{\sqrt{n}+1}{\ell}. \end{aligned} \tag{3.14}$$

A comparison with (2.9) shows that (3.13) is only asymptotically optimal, but the prior (3.10) gives us the flexibility for the analysis of the constrained case. Since δ^* is the Bayes estimate on the interval $[0,1]$, it follows that for any estimate δ

$$\begin{aligned} \sup_{\theta\in[a,b]} R_{sq}(\delta,\theta) &\geq \int_a^b R_{sq}(\delta,t)w_{m,\ell}(t)dt \\ &= \int_0^1 R_{sq}(\delta,t)w_{m,\ell}(t)dt - \Big(\int_0^a + \int_b^1\Big) R_{sq}(\delta,t)w_{m,\ell}(t)dt \\ &\geq \int_0^1 R_{sq}(\delta^*,t)w_{m,\ell}(t)dt - \Big(\int_0^a + \int_b^1\Big) \frac{w_{m,\ell}}{t(1-t)}(t)dt \\ &= \frac{1}{n+\sqrt{n}} - \Big(\int_0^a + \int_b^1\Big) \frac{w_{m,\ell}(t)}{t(1-t)}dt. \end{aligned} \tag{3.15}$$

The remaining integrals are now estimated similarly as in the proof of Lemma 3.1 using the non symmetric beta-prior. We set $\alpha := (a+b)/2$ and

$$m := \alpha(\sqrt{n}-2)+1, \quad \ell := (1-\alpha)(\sqrt{n}-2)+1. \tag{3.16}$$

Observing that α is the point, where the function $t^{m-1}(1-t)^{\ell-1}$ attains its unique maximum, and setting $s := \sqrt{n}-2$ we conclude with Lemma A.1 that

$$\int_0^a t^{m-1}(1-t)^{\ell-1}dt \le \frac{1}{n^2}\int_0^1 t^m(1-t)^\ell dt \tag{3.17}$$

for sufficiently large $n \in \mathbb{N}$. The same bound can be established for the integral over the interval $[b,1]$. Finally, a combination of (3.15) with (3.17) yields

$$\sup_{x\in[a,b]} R_{sq}(\delta,\theta) \ \ge\ \frac{1}{n+\sqrt{n}} - 2\frac{1}{n^2} \ =\ \frac{1}{n}(1+O(n^{-1/2}))$$

for any estimate δ, which gives the lower bound for (3.9).

We now turn to the proof of the estimate (3.8). The analysis of the quadratic loss for the interval $[0,b]$ heavily depends on a comparison with the normalized quadratic loss. The upper bound follows by using the estimate $\delta_k^0 = k/n$, and (2.9) gives for any $\theta \in [0,b]$

$$R_{qu}(\delta^0,\theta) = \theta(1-\theta)\,R_{sq}(\delta^0,\theta) = \theta(1-\theta)\frac{1}{n} \le \frac{b(1-b)}{n},$$

(note that $b \le \frac{1}{2}$). For deriving the lower bound we note that we have for any estimate δ and any $0 < \varepsilon < b-a$

$$\sup_{\theta\in[a,b]} R_{qu}(\delta,\theta) \ \ge\ (b-\varepsilon)(1-b-\varepsilon) \sup_{\theta\in[b-\varepsilon,b]} R_{sq}(\delta,\theta).$$

From (3.9) we know that the last factor is asymptotically at least $1/n(1+O(n^{-1/2}))$. Since $\varepsilon > 0$ may be arbitrarily small, the proof is complete. – This short proof, however, does not provide a rate of convergence for improving (3.8) $\square$

Theorem 3.3 *If $0 \le a < b \le 1$, then we have for the Kullback–Leibler distance*

$$\inf_\delta \sup_{\theta\in[a,b]} R_{KL}(\delta,\theta) = \frac{1}{2n}(1+o(1)).$$

A detailed proof of this result will be given in Appendix B. The main idea is to observe that the beta-prior (3.10) yields

$$\delta^{m,\ell}(k) = \frac{k+m+1}{n+m+\ell+2}.$$

as Bayes estimate. For this estimate a (uniform) risk of the form

$$\frac{1}{2n}(1+o(1))$$

can be verified in the subinterval $[\varepsilon, 1-\varepsilon]$ for any $\varepsilon > 0$. Thus we have a nearly constant Bayes risk in the actual domain and obtain the minimax value by standard arguments.

Remark 3.4 Marchand and MacGibbon (2000) showed numerically that the ratio of the linear minimax and minimax risk is close to one. Their explicit representation of the linear minimax rules [see Theorems 3.5 and 3.9 in Marchand and MacGibbon (2000)] and the results of the present paper show that the linear minimax estimates for quadratic and standardized quadratic loss also achieve the global asymptotic minimax risk in the case of a restricted parameter space.

Remark 3.5 The results show that the maximum risk with respect to the quadratic loss function can only be diminished asymptotically by additional knowledge about the probability of success, if the parameter space is restricted by that knowledge to an interval, which does not contain the center 1/2. For the two other risk functions additional knowledge regarding the location of the probability of success does not decrease the risk asymptotically. The arguments also show that the truncated estimators

$$\delta_k^{\frac{1}{2}\sqrt{n}} \cdot I\{a \leq \tfrac{k}{n} \leq b\} + a \cdot I\{\tfrac{k}{n} < a\} + b \cdot I\{\tfrac{k}{n} > b\}$$
$$\delta_k^{0} \cdot I\{a \leq \tfrac{k}{n} \leq b\} + a \cdot I\{\tfrac{k}{n} < a\} + b \cdot I\{\tfrac{k}{n} > b\}$$

and

$$\delta_k^{KL} \cdot I\{a \leq \tfrac{k}{n} \leq b\} + a \cdot I\{\tfrac{k}{n} < a\} + b \cdot I\{\tfrac{k}{n} > b\}$$

are asymptotically minimax rules; see also Charras and van Eeden (1991). We finally note that for the quadratic loss the linear minimax estimate takes values in the interval $[a, b]$, if $b - a$ is sufficiently large. In this case no truncation is required.

Remark 3.6 As pointed out by a referee it might be of interest to have some intuitive explanation of our results, which state that the location of the point 1/2 (with respect to the interval $[a, b]$) plays such an important role on the asymptotic minimax risk. For the quadratic loss with an unconstrained parameter space it is well known [see e.g. Lehmann (1983) or Bickel and Doksum (1977)] that the minimax estimate has only a smaller risk than the classical UMVU rule $\delta_k^0 = k/n$ in a neighbourhood $(-c_n + 1/2, 1/2 + c_n)$ of the point 1/2 which shrinks (i.e. $c_n \to 0$) to the point 1/2 for an increasing sample size. The reason for this fact is that the risk function of δ^0 is given by $\theta(1-\theta)/n$, which attains its maximum $1/(4n)$ at $\theta = 1/2$, Consequently, if squared error loss and a restricted parameter space $\Theta = [a, b]$ are considered, the asymptotic minimax risk remains unchanged, if and only if $1/2 \in [a, b]$. Note also that $\theta(1-\theta)/n$ is the optimal bound of the Cramér-Rao inequality for unbiased estimators of θ, and that the normalized squared error criterion takes into account the different size of this bound for different values of θ. As a consequence there exists no dominating value ϑ for the risk function of the UMVU rule δ^0 with respect to the normalized quadratic loss, and such phenomenon cannot be observed.

The argument for entropy loss function is similar using the expansion

$$\log(1 + x) = x - x^2/2 + o(x^2),$$

that is

$$\begin{aligned} p \log \frac{p}{q} + (1-p) \log \frac{1-p}{1-q} &= -p \log\Big(1 + \frac{q-p}{p}\Big) - (1-p) \log\Big(1 - \frac{q-p}{1-p}\Big) \\ &= \frac{(q-p)^2}{2p(1-p)} + o\Big(\frac{(q-p)^2(1-2p)}{p^2(1-p)^2}\Big). \end{aligned}$$

Consequently, we expect to observe the same phenomena for the entropy loss as found for the normalized quadratic loss. Theorems 3.1 – 3.3 make these heuristical arguments rigorous.

Remark 3.7 In the unrestricted case the parameters β in the optimal estimators for the squared error loss and the normalized squared error loss differ by $\sqrt{n}/2$. The difference in the resulting risk, however, is only a portion of order $n^{-1/2}$. Now a restriction of the probability θ may induce a shift of the parameter β in such a way that the difference between the two loss functions becomes less relevant for the choice of the estimator.

The behavior of the Kullback–Leibler distance is closer to that of the normalized squared error loss function. It is remarkable that the risk is very insensitive to the parameters β in the estimator as long as we stay in the interior of the interval $[0, 1]$ and $\beta \le n^{1/4}$. It is an effect of the boundary that usually parameters β close to 1/2 are chosen. In this context we note (without proof) that Theorem 3.3 can be improved if the boundary is excluded: *If* $0 < a < b < 1$, *then*

$$\inf_{\delta} \sup_{\theta \in [a,b]} R_{KL}(\delta, \theta) = \frac{1}{2n}(1 + O(n^{-1})).$$

4 Constrained minimax estimation of multinomial probabilities

In this section we study the problem of minimax estimation for the parameters of a multinomial distribution under certain constraints. As a by-product we also obtain some generalizations of the results in Section 3 to more general parameter spaces $\Theta \subset [0, 1]$. To be precise, let $n, d \in \mathbb{N}$ and assume that $X = (X_0, \ldots, X_d)^T$ is a random vector with probability law

$$P(X_i = k_i;\ i = 0, \ldots, d) = M_{n,k}(\theta) := n! \prod_{i=0}^{d} \frac{\theta_i^{k_i}}{k_i!}\ , \tag{4.1}$$

whenever $\sum_{i=0}^{d} k_i = n$ and 0 otherwise. Here the vector of probabilities $\theta = (\theta_0, \ldots, \theta_d)^T$ is contained in the d-dimensional simplex

$$\Delta := \left\{ (x_0, \ldots, x_d)^T \in [0, 1]^{d+1} \mid \sum_{i=0}^{d} x_i = 1 \right\}. \tag{4.2}$$

Throughout this section we let

$$\delta = (\delta^0, \ldots, \delta^d)^T\ :\ \left\{ (k_0, \ldots, k_d) \in \mathbb{N}_0^{d+1} \,\middle|\, \sum_{i=0}^{d} k_i = n \right\} \longrightarrow \Delta$$

denote a nonrandomized estimate of θ, and we write for the sake of simplicity

$$\delta_k = \delta(k) = (\delta^0(k), \ldots, \delta^d(k))^T = (\delta_k^0, \ldots, \delta_k^d)^T.$$

In the unconstrained case $\theta \in \Delta$ much effort has been devoted to the problem of minimax estimation of the vector θ with respect to quadratic and normalized quadratic loss functions [see e.g. Steinhaus (1957), Trybula (1958, 1986), Olkin and Sobel (1977), Wilczynski (1985), He (1990) among many others]. Braess, Forster, Sauer, and Simon (2002) consider the multivariate entropy loss and extend the lower bound of Cover (1972) to the multivariate case. In the present section we consider the problem of minimax estimation of a vector of constrained multinomial probabilities with respect to the loss functions

$$
\begin{aligned}
(4.3)\qquad L_{qu}(\delta,\theta) &= \sum_{i=0}^{d}(\delta^i-\theta_i)^2,\\
(4.4)\qquad L_{sq}(\delta,\theta) &= \sum_{i=0}^{d}\frac{(\delta^i-\theta_i)^2}{\theta_i},\\
(4.5)\qquad L_{KL}(\delta,\theta) &= \sum_{i=0}^{d}\theta_i\log\frac{\theta_i}{\delta^i}\,.
\end{aligned}
$$

The corresponding risks are denoted by R_{qu}, R_{sq}, and R_{KL}, respectively. Note that

$$L_{sq}(\delta,\theta) = (\bar\delta-\bar\theta)^T\Sigma^{-1}(\bar\delta-\bar\theta)$$

where $\Sigma = \mathrm{diag}(\theta_1,\dots,\theta_d)-(\theta_i\theta_j)_{i,j=1}^d$ is the Fisher information matrix of $\bar\theta$ and the vectors $\bar\delta,\bar\theta$ are obtained from the corresponding quantities δ, θ by omitting the first component. Consequently, (4.4) is the multivariate analogue of the normalized loss (2.4). The minimax estimators in the unconstrained case for the quadratic and normalized quadratic loss functions are given by

$$(4.6)\qquad \delta^i_{qu}(k) = \frac{k_i+\sqrt{n}/(d+1)}{n+\sqrt{n}},\quad i=0,\dots,d,$$

[see Steinhaus (1957)] and

$$(4.7)\qquad \delta^i_{sq}(k) = \frac{k_i}{n}\,,\quad i=0,\dots,d,$$

[see Olkin and Sobel (1979)], respectively, where the vector $k=(k_0,\dots,k_d)\in\mathbb{N}_0^{d+1}$ satisfies $\sum_{i=0}^d k_i = n$. The rules (4.6) and (4.7) have the form

$$(4.8)\qquad \delta^i_\beta(k) = \frac{k_i+\beta}{n+(d+1)\beta},\quad i=0,\dots,d;$$

and are therefore multivariate add-β-rules. The corresponding minimax risks with respect to the unconstrained parameter space are given by

$$
\begin{aligned}
(4.9)\qquad \inf_\delta\sup_{\theta\in\Delta}R_{qu}(\delta,\theta) &= \sup_{\theta\in\Delta}R_{qu}(\delta_{qu},\theta) = \frac{d}{d+1}\,\frac{n}{(n+\sqrt{n})^2}\,,\\
(4.10)\qquad \inf_\delta\sup_{\theta\in\Delta}R_{sq}(\delta,\theta) &= \sup_{\theta\in\Delta}R_{sq}(\delta_{sq},\theta) = \frac{d}{n}\,,\\
(4.11)\qquad \inf_\delta\sup_{\theta\in\Delta}R_{KL}(\delta,\theta) &= \frac{d}{2n}(1+o(1)),
\end{aligned}
$$

respectively [see Braess and Sauer (2003) for the last estimate].

In the following we establish the asymptotic minimax risks for the estimation of constrained multinomial probabilities, where the parameter θ is known to be contained in a subset $\Theta \subset \Delta$. Here the analysis is more involved since there are no simple generalizations of the inequalities (3.6) and (3.7).

Theorem 4.1 *(a) If $\Theta \subset \Delta$ contains a neighborhood of the point $\left(\frac{1}{d+1}, \ldots, \frac{1}{d+1}\right)^T$, then*

$$\inf_{\delta} \sup_{\theta \in \Theta} R_{qu}(\delta, \theta) = \frac{d}{d+1} \frac{n}{(n+\sqrt{n})^2} (1 + O(n^{-1})). \tag{4.12}$$

(b) If $\Theta \subset \Delta$ contains an open set, then

$$\inf_{\delta} \sup_{\theta \in \Theta} R_{sq}(\delta, \theta) = \frac{d}{n}(1 + o(1)), \tag{4.13}$$

$$\inf_{\delta} \sup_{\theta \in \Theta} R_{KL}(\delta, \theta) = \frac{d}{2n}(1 + o(1)). \tag{4.14}$$

Proof. (a) Since the upper bound is clear from (4.9), we turn to the proof of the lower bound. Priors of the form

$$w_m(t) := c_m \prod_{i=0}^{d} t_i^{m_i} \tag{4.15}$$

where $m = (m_1, \ldots, m_d)$ and c_m is a normalization factor, will be appropriate in all cases. Here we consider the Bayes risk for priors with $m_i = \ell$ for all i. It is well-known [see e.g. Steinhaus (1957)] that the Bayes estimate with respect to the prior w_m with $m = (\ell, \ldots, \ell)$ is the multivariate add-β-rule (4.8) with $\beta = \ell + 1$. This fact is independent of the dimension. Therefore, the rule δ_{qu} as given by (4.6) is the Bayes estimate with respect to the prior w_m if we choose $m_i := \sqrt{n}/(d+1) - 1$ for all i. We also recall that $R_{qu}(\delta_{qu}, \cdot)$ is a constant function given by the right hand side of (4.9) [see Steinhaus (1957)]. Now we can proceed as in the proof of Theorem 3.1. We note that $R_{qu}(\delta, \theta) \leq d+1$ holds for all pairs (δ, θ), and we only have to apply Lemma A.2 with $\alpha = \frac{1}{d+1}(1, 1, \ldots, 1)^T$ instead of Lemma A.1 to complete the proof.

(b) A proof of (4.13) proceeds in the same manner and is a generalization of the proof of (3.9) for Theorem 3.2. Let α be an interior point of Θ. In particular, all components of α are positive. Set $m_i := (\sqrt{n} - d - 1)\alpha_i + 1$ for $i = 0, 1, \ldots, d$. Obviously, $\sum_{i=0}^{d} m_i = \sqrt{n}$. From Lemma A.3 it follows that the prior (A.1) leads to a Bayes risk that has the correct asymptotic rate, i.e. $\frac{d}{n}(1 + o(1))$. Moreover, $R_{sq}(\delta, \theta) \leq (d+1)/\prod_{j=0}^{d} \theta_j$ holds for all pairs (δ, θ). Now we also proceed along the lines of the proof in the univariate case, we only have to apply Lemma A.2 instead of Lemma A.1 to complete the proof of (4.13).

The proof of (4.14) is similar to the proof of Theorem 3.3 after the multidimensional case has been reduced to a one-dimensional by Lemma 6 in Braess and Sauer (2003). It is abandoned here. $\square$

Finally we deal with the case which was excluded in the preceding theorem.

Theorem 4.2 *Let $\Theta \subset \Delta$, and assume that Θ is the closure of its interior points. Then*

$$\inf_{\delta} \sup_{\theta\in\Theta} R_{qu}(\delta,\theta) = \frac{1}{n} \sup_{\theta\in\Theta} \sum_{i=0}^{d} \theta_i(1-\theta_i)(1+o(1)) \,. \tag{4.16}$$

Note that (4.16) is a generalization of (4.12) since

$$\sup_{\theta\in\Theta} \sum_{i=0}^{d} \theta_i(1-\theta_i) = \frac{d}{d+1} = \sup_{\theta\in\Delta} \sum_{i=0}^{d} \theta_i(1-\theta_i) \,,$$

whenever the set Θ contains the point $(\frac{1}{d+1}, \ldots, \frac{1}{d+1})^T$.

Proof of Theorem 4.2. For establishing the upper bound, we consider the minimax estimator with respect to the normalized quadratic loss function L_{sq} given in (4.7)

$$\delta^i_{sq}(k) = \frac{k_i}{n}.$$

The resulting risk is

$$R_{qu}(\delta_{sq},\theta) = \frac{1}{n} \sum_{i=0}^{d} \theta_i(1-\theta_i), \tag{4.17}$$

and by taking the supremum we obtain the upper bound.
We turn to the verification of the bound from below. Given $\varepsilon > 0$, let α be an interior point of Θ such that

$$\sum_{i=0}^{d} \alpha_i(1-\alpha_i) \geq \sup_{\theta\in\Theta} \sum_{i=0}^{d} \theta_i(1-\theta_i) - \varepsilon.$$

We consider the prior (4.15) with

$$m_i := \alpha_i s, \quad i = 0,1,\ldots,d, \quad s := \sqrt{n} - d - 1. \tag{4.18}$$

The corresponding Bayes estimate for the quadratic loss function is given by

$$\delta^{*i}(k) = \frac{k_i + m_i + 1}{n + |m| + d + 1} \,,$$

where we used the notation $|m| = \sum_{i=0}^{d} m_i$. Note that $\sum_{i=0}^{d}(m_i+1) = \sqrt{n}$, and a straightforward calculation analogous to (A.4) yields

$$\begin{aligned} R_{qu}(\delta^*,\theta) &= \frac{1}{(n+\sqrt{n})^2} \sum_{i=0}^{d} \Big\{ (m_i+1)^2 - 2(|m|+d+1)(m_i+1)\theta_i + n\theta_i \Big\} \\ &= \frac{1}{(n+\sqrt{n})^2} \sum_{i=0}^{d} \Big\{ (m_i+1)^2 - 2\sqrt{n}(m_i+1)\theta_i + n\theta_i \Big\}. \end{aligned}$$

Next we note that
$$\frac{\int_\Delta w_m(t)t_i\,dt}{\int_\Delta w_m(t)\,dt} = \frac{m_i+1}{\sum_{i=0}^d m_i + d + 1} = \frac{m_i+1}{\sqrt{n}}\,.$$
Hence,
$$\begin{aligned}\int_\Delta R_{qu}(\delta^*,t)w_m(t)\,dt &= \frac{1}{(n+\sqrt{n})^2}\sum_{i=0}^d \Big\{n - \sum_{i=0}^d (m_i+1)^2\Big\} \\ &= \frac{1}{(n+\sqrt{n})^2}\sum_{i=0}^d \Big\{n - \sum_{i=0}^d m_i^2 - 2|m| - d - 1\Big\} \\ &\geq \frac{1}{(n+\sqrt{n})^2}\sum_{i=0}^d \Big\{n - \sum_{i=0}^d \alpha_i^2(\sqrt{n})^2 - 2\sqrt{n}\Big\} \\ &= \frac{n}{(n+\sqrt{n})^2}\sum_{i=0}^d \Big\{1 - \sum_{i=0}^d \alpha_i^2\Big\}(1+O(n^{-1/2})).\end{aligned}$$
Since $\alpha \in \Delta$, it follows that $1-\sum_{i=0}^d \alpha_i^2 = \sum_{i=0}^d \alpha_i(1-\alpha_i)$, and the proof can be completed as the proof of Theorem 4.1a. □

A Appendix: Auxiliary results

A.1 Two Lemmas

Lemma A.1 *If $0<a<\alpha<1$, then the estimate*
$$\begin{aligned}\int_0^a t^{\alpha s}(1-t)^{(1-\alpha)s}dt &\leq (s+2)^{-4}\int_0^1 t^{\alpha s+1}(1-t)^{(1-\alpha)s+1}dt \\ &\leq (s+2)^{-4}\int_0^1 t^{\alpha s}(1-t)^{(1-\alpha)s}dt\end{aligned}$$
holds for sufficiently large s.

Proof. We choose $\gamma \in (a,\alpha)$. The function $t \mapsto t^{\alpha s}(1-t)^{(1-\alpha)s}$ attains its (unique) maximum at $t=\alpha$ and consequently we have $\lambda := a^\alpha(1-a)^{(1-\alpha)}/\gamma^\alpha(1-\gamma)^{(1-\alpha)} < 1$. The monotonicity of this function on $(0,\alpha)$ also implies
$$\begin{aligned}\int_0^a t^{\alpha s}(1-t)^{(1-\alpha)s}dt &\leq a[a^\alpha(1-a)^{(1-\alpha)}]^s = a\lambda^s[\gamma^\alpha(1-\gamma)^{(1-\alpha)}]^s \\ &\leq \frac{a}{\alpha-\gamma}\,\lambda^s\int_\gamma^\alpha t^{\alpha s}(1-t)^{(1-\alpha)s}dt \\ &\leq \frac{a}{\alpha-\gamma}\,\frac{1}{\alpha(1-\gamma)}\,\lambda^s\int_\gamma^\alpha t^{\alpha s+1}(1-t)^{(1-\alpha)s+1}dt \\ &\leq \frac{a}{\alpha-\gamma}\,\frac{1}{\alpha(1-\gamma)}\,\lambda^s\int_0^1 t^{\alpha s+1}(1-t)^{(1-\alpha)s+1}dt.\end{aligned}$$

The first inequality in the assertion now follows from $(s+2)^4\lambda^s \to 0$ as $s \to \infty$, and the second one is obvious. $\square$

An extension of the lemma above is required for the analysis of the multivariate case.

Lemma A.2 *Assume that $\alpha = (\alpha_0, \dots, \alpha_d)$ is an interior point of the set $\Theta \subset \Delta$ with Δ being defined in (4.2). Let Θ^c denote the complement of the set Θ in Δ. With the notation $\phi(t) := \prod_{i=0}^d t_i^{\alpha_i}$, we have for sufficiently large s:*

$$\int_{\Theta^c} \phi(t)^s dt \le (s+d+1)^{-4} \int_\Delta \phi(t)^s \prod_{j=0}^d t_j dt \le (s+d+1)^{-4} \int_\Delta \phi(t)^s dt.$$

Proof. Set $r := \phi(\alpha)$ and note that the function ϕ attains its unique maximum at the point α. By compactness, we therefore obtain

$$\lambda := \frac{1}{r} \sup_{t \in \Theta^c} \phi(t) < 1.$$

Now consider the set

$$T := \{t \in \Delta; \phi(t) \ge \lambda^{1/2} r\}$$

and let $|\Theta^c|$ and $|T|$ denote the Lebesgue measure of Θ^c and T, respectively. The product $\prod_{j=0}^d t_j$ is positive on the compact set Θ^c. With these preparations we obtain the following estimates for the integral under consideration

$$\begin{aligned}
\int_{\Theta^c} \phi(t)^s dt &\le |\Theta^c| \sup_{t\in\Theta^c}\{\phi(t)^s\} = |\Theta^c|\,(r\lambda)^s \\
&\le |\Theta^c|\,\lambda^{s/2}\,\frac{1}{|T|}\int_T \phi(t)^s dt \\
&\le \frac{|\Theta^c|}{|T|} \sup_{t\in\Theta^c}\Big\{\prod_{j=0}^d t_j^{-1}\Big\}\ \lambda^{s/2} \int_T \phi(t)^s \prod_{j=0}^d t_j\,dt \\
&\le \frac{|\Theta^c|}{|T|} \sup_{t\in\Theta^c}\Big\{\prod_{j=0}^d t_j^{-1}\Big\}\ \lambda^{s/2} \int_\Delta \phi(t)^s \prod_{j=0}^d t_j\,dt\,.
\end{aligned}$$

Now the first assertion follows from $(s+d+1)^4\lambda^{s/2} \to 0$ as $s \to \infty$, and the second inequality is obvious. $\square$

A.2 A suboptimal Bayes risk

Lemma A.3 *Let $m_i > 0,\ i = 0, 1, \dots, d$, $m = (m_0, \dots, m_d)$ and*

$$w_m(t) := c_m \prod_{j=0}^d t_j^{m_j}, \qquad \int_\Delta w_m(t)dt = 1, \tag{A.1}$$

denote the (generalized) beta-prior. Then the Bayes estimate with respect to the normalized risk (4.4) and the prior (A.1) is

$$\delta^{*i}(k) = \frac{k_i + m_i}{n + |m|}\,, \tag{A.2}$$

where $|m| := \sum_{i=0}^d m_i$. *If moreover* $|m| = \sqrt{n}$, *then the risk of* δ^* *is given by (A.4) below and the Bayes risk is*

$$\int_\Delta R_{sq}(\delta^*, t) w_m(t) dt = \frac{d}{n + \sqrt{n}}\,. \tag{A.3}$$

Proof. Using the notation $t = (t_0, \ldots, t_d)$ we compute the integral under consideration

$$\begin{aligned}
&\int_\Delta \sum_k M_{n,k}(t) \sum_{i=0}^d \frac{(t_i - \delta^i(k))^2}{t_i} \prod_{j=0}^d t_j^{m_j}\, dt \\
&= \sum_k \frac{n!}{k_0! \ldots k_d!} \sum_{i=0}^d \int_\Delta (t_i - \delta^i(k))^2\, t_i^{m_i + k_i - 1} \prod_{j \neq i} t_j^{m_j + k_j}\, dt \\
&= \sum_k \frac{n!}{k_0! \ldots k_d!} \sum_{i=0}^d \Big\{ \delta^i(k)^2\, \frac{\prod_{j=0}^d \Gamma(m_j + k_j + 1)}{(m_i + k_i)\Gamma(|m| + n + d)} \\
&\qquad\qquad -2\delta^i(k)\, \frac{\prod_{j=0}^d \Gamma(m_j + k_j + 1)}{\Gamma(|m| + n + d + 1)} + \text{const} \Big\}.
\end{aligned}$$

When the minimum over all $\delta(k)$ is determined, we may add a multiple of $\sum_{i=0}^d \delta^i(k) - 1$ and obtain (A.2) by looking for a root of the gradient.

Note that $\delta^{*i}(k)$ depends only on the component k_i. Therefore, we can use the reduction to one-dimensional expressions as given by Lemma 6 of Braess and Sauer (2003). *For any set of functions* $G_j \,:\, [0,1] \times \mathbb{N} \to \mathbb{R}$ *we have*

$$\sum_k M_{n,k}(\theta) \sum_{i=0}^d G_i\left(\theta_i, k_i\right) = \sum_{i=0}^d \sum_{j=0}^n B_{n,j}\left(\theta_i\right)\, G_i\left(\theta_i, j\right).$$

The risk for the Bayes estimate is now evaluated

$$\begin{aligned}
R_{sq}(\delta^*, \theta) &= \sum_k M_{n,k}(\theta) \sum_{i=0}^d \frac{1}{\theta_i} (\theta_i - \delta^i(k))^2 \\
&= \sum_{i=0}^d \sum_{j=0}^n B_{n,j}(\theta_i) \frac{1}{\theta_i} \Big(\theta_i - \frac{j + m_i}{n + |m|} \Big)^2.
\end{aligned}$$

The sums over Bernstein polynomials and quadratic expressions in j yield quadratic expressions in θ_i,

$$R_{sq}(\delta^*, \theta) = \sum_{i=0}^d \frac{1}{\theta_i} \Big\{ (\theta_i - \frac{m_i}{n + |m|} - \frac{n}{n + |m|}\theta_i)^2 + \frac{n}{(n + |m|)^2}\theta_i(1 - \theta_i) \Big\}$$

$$= \frac{1}{(n+|m|)^2}\sum_{i=0}^{d}\frac{1}{\theta_i}\Big\{(|m|\theta_i - m_i)^2 + n\theta_i(1-\theta_i)\Big\}.$$

Next, we restrict ourselves to the case $|m| = \sqrt{n}$ to obtain

$$R_{sq}(\delta^*, \theta) = \frac{1}{(n+\sqrt{n})^2}\sum_{i=0}^{d}\frac{1}{\theta_i}\Big\{m_i^2 - 2|m|m_i\theta_i + n\theta_i\Big\}$$

$$= \frac{1}{(n+\sqrt{n})^2}\Big\{n(d-1) + \sum_{i=0}^{d}\frac{m_i^2}{\theta_i}\Big\}. \tag{A.4}$$

Recall that $\int_\Delta \frac{1}{t_i}\prod_j t_j^{m_j}\,dt/\int_\Delta \prod_j t_j^{m_j}\,dt = (|m|+d)/m_i$, and we have

$$\int_\Delta R_{sq}(\delta^*, \theta) w_m(t) dt = \frac{1}{(n+\sqrt{n})^2}\{n(d-1) + \sum_{i=0}^{d} m_i\,(|m|+d)\}$$

$$= \frac{d}{n+\sqrt{n}},$$

which completes the proof of the lemma. □

B Appendix: Proof of Theorem 3.3

The proof of Theorem 3.3 requires several preparations. While the Bayes risk for priors of the form (3.10) was known for the squared loss and the normalized squared loss, it has to be established here for the Kullback–Leibler distance.

Given $f \in C[0,1]$ let $B_n[f]$ denote its n-th Bernstein polynomial

$$B_n[f](x) := \sum_{k=0}^{n} B_{n,k}(x) f(\frac{k}{n}).$$

Braess and Sauer (2003) established *lower bounds* for $f - B_n[f]$, where

$$f(x) := -x\log x + (1-x)\log(1-x). \tag{B.1}$$

However, for our purposes upper bounds are required. Fortunately they are more easily obtained since we can abandon the boundary points 0 and 1 and the trouble that they cause.

Lemma B.1 *Let f be defined by (B.1), and $0 < a < b < 1$. Then*

$$f(x) - B_n[f](x) \le \frac{1}{2n} + \frac{c_0}{n^2} \quad \text{for all } a \le x \le b,$$

with c_0 being a constant that depends only on a and b.

Proof. Given $x_0 \in [a, b]$, let Q_3 be the Taylor polynomial

$$Q_3(x) = f(x_0) + f'(x_0)(x - x_0) - \frac{1}{2x_0(1 - x_0)}(x - x_0)^2 + \frac{1}{3!}f'''(x_0)(x - x_0)^3.$$

Here we only give an explicit expression for the second derivative since the associated term is the crucial one. Let $a_1 := a/2$ and $b_1 := (b + 1)/2$. By Taylor's remainder formula we have

$$Q_4(x) = Q_3(x) + \frac{c'}{4!}(x - x_0)^4 \geq f(x) \tag{B.2}$$

for $a_1 \leq x \leq b_1$ if we set $c' = \min_{a_1 \leq t \leq b_1}\{f^{(4)}(t)\}$. After reducing c' by a finite amount, we know that (B.2) holds for all $x \in [0, 1]$. In particular, a compactness argument shows that $|c'|$ can be bounded by a constant that depends only on a and b.

The monotonicity of the Bernstein operator $f \mapsto B_n[f]$ and the inequality (B.2) imply that $B_n[f](x) \leq B_n[Q_4](x)$. We will make use of this fact at $x = x_0$. By Proposition 4 of Braess and Sauer (2003) or Lorentz (1952) we know that:

$$\begin{aligned}
B_n[1](x_0) &= 1, \\
B_n[(x - x_0)](x_0) &= 0, \\
B_n[(x - x_0)^2](x_0) &= \frac{x_0(1 - x_0)}{n}, \\
B_n[(x - x_0)^3](x_0) &= \frac{x_0(1 - x_0)}{n^2}(1 - 2x_0), \\
B_n[(x - x_0)^4](x_0) &= 3\,\frac{x_0^2(1 - x_0)^2}{n^2} + \frac{x_0(1 - x_0)}{n^3}[1 - 6x_0(1 - x_0)].
\end{aligned}$$

The cubic and the quartic terms give only rise to contributions of order $O(n^{-2})$ and

$$B_n[f](x_0) \leq B_n[Q_4](x_0) = f(x_0) - \frac{x_0(1 - x_0)}{2n\, x_0(1 - x_0)} + c''\frac{1}{n^2}\,.$$

The difference $f(x_0) - B_n[f](x_0)$ yields the required estimate at $x = x_0$. $\square$

Lemma B.2 *Let $m, \ell > 0$. Then the Bayes estimate with respect to the Kullback–Leibler distance (2.5) and the prior $w_{m-1,\ell-1}$ defined in (3.10) is given by the rule $\delta^{m,\ell}$ in (3.11). If moreover $m + \ell = n^{1/4}$, then the risk of $\delta^{m,\ell}$ implies*

$$R_{KL}(\delta^{m,\ell}, \theta) \geq \frac{1}{2n} - \frac{c_1}{n^2} \quad \textit{for } a \leq x \leq b \tag{B.3}$$

with c_1 depending only on a and b. If $0 < \alpha < 1$, $m = \alpha n^{1/4}$, and $\ell = (1 - \alpha)n^{1/4}$, then the Bayes risk satisfies

$$\int_0^1 R_{KL}(\delta^{m,\ell}, t) w_{m-1,\ell-1}(t)dt \geq \frac{1}{2n} - \frac{c_2}{n^2}\,. \tag{B.4}$$

with c_2 depending only on α.

Proof. (1) When the Bayes estimate is determined, we may ignore the terms that do not depend on δ,

$$\begin{aligned}
&\int_0^1 R_{KL}(\delta^{m,\ell}, t) w_{m-1,\ell-1}(t) dt \\
&\quad = c_{m,\ell} \sum_{k=0}^{n} \int_0^1 t^{m+k-1}(1-t)^{\ell+n-k-1} \, [t \log \frac{1}{\delta_k} + (1-t) \log \frac{1}{1-\delta_k}] \, dt \\
&\qquad + const \\
&\quad = c_{m,\ell} \sum_{k=0}^{n} \binom{n}{k} \frac{\Gamma(m+k)\Gamma(\ell+n-k)}{\Gamma(m+\ell+n+1)} \, [(m+k) \log \frac{1}{\delta_k} + (\ell+n-k) \log \frac{1}{1-\delta_k}] \\
&\qquad + const.
\end{aligned}$$

Each parameter δ_k enters only into one summand and the minimum is attained if $\frac{m+k}{\delta_k} - \frac{\ell+n-k}{1-\delta_k} = 0$ which yields (3.11) as Bayes estimate.

(2) Following Braess and Sauer (2003) we determine the risk for $n-1$ instead of n. Recalling (B.1) we find by a shift of indices

$$\begin{aligned}
R_{KL,n-1}(\delta, \theta) &= \sum_{k=0}^{n-1} \binom{n-1}{k} \theta^k (1-\theta)^{n-1-k} \Big[\theta \log \frac{\theta}{\delta_k} + (1-\theta) \log \frac{1-\theta}{1-\delta_k}\Big] \\
&= \sum_{k=0}^{n} \binom{n}{k} \theta^k (1-\theta)^{n-k} \Big[\frac{k}{n} \log \frac{1}{\delta_{k-1}} + \frac{n-k}{n} \log \frac{1}{1-\delta_k}\Big] - f(\theta) \\
&= \frac{1}{n} \sum_{k=0}^{n} B_{n,k}(\theta) \Big[k \log \frac{k/n}{\delta_{k-1}} + (n-k) \log \frac{(n-k)/n}{1-\delta_k}\Big] + (B_n[f] - f)(\theta) \\
&=: \Delta R_{KL}(\delta, \theta) + (B_n[f] - f)(\theta). \qquad \text{(B.5)}
\end{aligned}$$

Only the first term depends on δ. We evaluate it for $\delta = \delta^{m,\ell}$ to obtain

$$\begin{aligned}
\Delta R_{KL}(\delta^{m,\ell}, \theta) &= \frac{1}{n} \sum_{k=0}^{n} B_{n,k}(\theta) \Big[k \log \frac{k/n}{(k-1+m)/(n+m+\ell-1)} \\
&\qquad\qquad + (n-k) \log \frac{(n-k)/n}{(n-k+\ell-1)/(n+m+\ell-1)}\Big] \\
&= \frac{1}{n} \sum_{k=0}^{n} B_{n,k}(\theta) \Big[-k \log \frac{k+m-1}{k} - (n-k) \log \frac{n-k+\ell-1}{n-k}\Big] \\
&\qquad + \log \frac{n+m+\ell-1}{n} \, .
\end{aligned}$$

The logarithmic terms can be estimated due to $z - \frac{z^2}{2} \le \log(1+z) \le z$ for $0 \le z \le 1$:

$$\Delta R_{KL}(\delta^{m,\ell}, \theta) \ge \frac{1}{n} \sum_{k=0}^{n} B_{n,k}(\theta) \Big[-(m-1) - (\ell-1)\Big] + \frac{m+\ell-1}{n} - \frac{1}{2} \Big(\frac{m+\ell-1}{n}\Big)^2$$

$$\geq \frac{1}{n} - \frac{1}{2}n^{-3/2}$$

if $m+\ell \leq n^{1/4}$. Combining this with (B.5) and recalling Lemma B.1 we obtain (B.3). – In particular we conclude from (B.3) and the cited upper estimate that $R_{KL}(\delta^{m,\ell},\cdot)$ is asymptotically a nearly constant function in the interior of the interval.

(3) Given $\alpha \in (0,1)$, set $a = \alpha/2$ and $b = (\alpha+1)/2$. Now (B.3) and Lemma A.1 yield

$$\begin{aligned}
\int_0^1 R_{KL}(\delta^{m,\ell},t)w_{m-1,\ell-1}(t)dt &\geq \int_a^b R_{KL}(\delta^{m,\ell},t)w_{m-1,\ell-1}(t)dt \\
&\geq \left(\frac{1}{2n} - \frac{c_1}{n^2}\right)\int_a^b w_{m-1,\ell-1}(t)dt \\
&\geq \left(\frac{1}{2n} - \frac{c_1}{n^2}\right)\left(1 - \frac{2}{n}\right). \qquad \text{(B.6)}
\end{aligned}$$

This proves (B.4), and the proof is complete. □

Now we are in a position to complete the

Proof of Theorem 3.3. We may assume that $0 < a$ and $b < 1$ since a reduction of the interval does not enhance the value of the risk. We know from the arguments in Remark 3.5 that the candidates for the best estimates satisfy

$$a \leq \delta_k \leq b, \quad k = 0,1,\ldots,n,$$

and we have

$$R_{KL}(\delta,\theta) = \theta\log\frac{\theta}{\delta} + (1-\theta)\log\frac{1-\theta}{1-\delta} \leq \log\frac{1}{a} + \log\frac{1}{1-b} \quad \forall\,\theta \in [0,1]. \qquad \text{(B.7)}$$

The rest of the proof proceeds as for the other loss functions; cf. (3.4). The integral with weight function $w_{m-1,\ell-1}$ over the full interval $[0,1]$ can be estimated from below by (B.6) and the integrals over $[0,a]$ and $[b,1]$ by (B.7) and Lemma A.1. □

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