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A multivariate normal approximation for the Dirichlet density and some applications

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Abstract

In this short note, we prove an asymptotic expansion for the ratio of the Dirichlet density to the multivariate normal density with the same mean and covariance matrix. The expansion is then used to derive an upper bound on the total variation between the corresponding probability measures and rederive the asymptotic variance of the Dirichlet kernel estimators introduced by Aitchison and Lauder (1985) and studied theoretically in Ouimet (2020). Another potential application related to the asymptotic equivalence between the Gaussian variance regression problem and the Gaussian white noise problem is briefly mentioned but left open for future research.

KEYWORDS:

Dirichlet distribution; asymptotic statistics; expansion; normal approximation; Gaussian approximation; multivariate normal; total variation; asymptotic variance; nonparametric statistics; smoothing; density estimation

1 | INTRODUCTION

For any $d \in \mathbb{N}$ and $\mathbf{v} \in \mathbb{R}^d$, let $\|\mathbf{v}\|_1 := \sum_{i=1}^d |v_i|$ denote the ℓ^1 norm and define the d -dimensional simplex as

$$\mathcal{S}_d := \{\mathbf{v} \in [0, 1]^d : \|\mathbf{v}\|_1 \leq 1\}. \quad (1)$$

Given the parameters $N \in \mathbb{N}$ and $(\alpha, \beta) \in (0, \infty)^{d+1}$, the Dirichlet $(N\alpha, N\beta)$ density function is defined by

$$K_{N, \alpha, \beta}(\mathbf{x}) = \frac{\Gamma(N\|\alpha\|_1 + N\beta)}{\Gamma(N\beta) \prod_{i=1}^d \Gamma(N\alpha_i)} \cdot (1 - \|\mathbf{x}\|_1)^{N\beta-1} \prod_{i=1}^d x_i^{N\alpha_i-1}, \quad \mathbf{x} \in \mathcal{S}_d. \quad (2)$$

The covariance matrix of the Dirichlet distribution is well-known to be $(N\|\alpha\|_1 + N\beta + 1)^{-1} \Sigma_r$, where

$$\Sigma_r := \text{diag}(\mathbf{r}) - \mathbf{r}\mathbf{r}^\top \quad \text{and} \quad \mathbf{r} := \frac{\alpha}{\|\alpha\|_1 + \beta}, \quad (3)$$

see, e.g., (Ng, Tian, & Tang 2011, p.39). By adapting Theorem 1 and Equation (21) in Tanabe and Sagae (1992), we also know that

$$\det(\Sigma_r) = \prod_{i=1}^{d+1} r_i \quad \text{and} \quad (\Sigma_r^{-1})_{ij} = \frac{1}{r_i} \mathbb{1}_{\{i=j\}} + \frac{1}{r_{d+1}}, \quad i, j \in \{1, 2, \dots, d\}, \quad (4)$$

where $r_{d+1} := 1 - \|\mathbf{r}\|_1 = \frac{\beta}{\|\alpha\|_1 + \beta}$.

The first goal of the paper (Theorem 1) is to establish an asymptotic expansion for the ratio of the Dirichlet density (2) to the multivariate normal density with the same mean and covariances, namely:

$$(N\|\alpha\|_1 + N\beta + 1)^{d/2} \phi_{\Sigma_r}(\delta_{\mathbf{x}}), \quad \mathbf{x} \in \mathbb{R}^d, \quad \text{where } \phi_{\Sigma_r}(\mathbf{y}) := \frac{\exp(-\frac{1}{2}\mathbf{y}^\top \Sigma_r^{-1} \mathbf{y})}{\sqrt{(2\pi)^d \det(\Sigma_r)}}, \quad (5)$$

and where

$$\delta_{\mathbf{x}} := (\delta_{1,x_1}, \delta_{2,x_2}, \dots, \delta_{d,x_d}) \quad \text{and} \quad \delta_{i,x_i} := \frac{x_i - r_i}{(N\|\alpha\|_1 + N\beta + 1)^{-1/2}}. \quad (6)$$

The second goal of the paper is to apply the asymptotic expansion to derive an upper bound on the total variation between the probability measures on $\mathbb{R}^d$ induced by (2) and (5), and to rederive the asymptotic variance of the Dirichlet kernel estimators in the context of density estimation for compositional data. These two applications are treated in Section 3.1 and Section 3.2, respectively. There could be many other potential applications, see for example the excellent survey by Mason and Zhou (2012) on quantile coupling inequalities.

In fact, the original motivation for the present paper was the PhD thesis of Huibin Zhou (Zhou 2004), in which a multi-resolution coupling methodology between beta and normal random variables is applied to prove the asymptotic equivalence between the Gaussian variance regression problem and the Gaussian white noise problem under Besov smoothness constraints (see also the related works of Brown and Low (1996), Brown and Zhang (1998), Grama and Nussbaum (1998), Grama and Nussbaum (1998), Brown, Cai, Low, and Zhang (2002), Rohde (2004), Carter (2006), Carter (2007), Reiß (2008), Cai and Zhou (2009), Golubev, Nussbaum, and Zhou (2010) and Meister and Reiß (2013)). In Zhou (2004), the main idea was that the information we get from the sampled observations $X_i \sim \text{Normal}(0, f(t_i))$, where the t_i 's form a fixed partition of $[0, 1]$ and f is an unknown density function, can be encoded using the (Gaussian) increments of a properly scaled Brownian motion with drift $t \mapsto \frac{1}{\sqrt{2}} \int_0^t \log f(s) ds$, and vice versa. Ultimately, the crucial step in the proof involves multiscale inductive quantile couplings (comparisons) between conditionally scaled chi-squared random variables (i.e., beta random variables) and Gaussian analogues, akin to the multiscale argument in Carter (2002) used to prove the asymptotic equivalence between the density estimation problem and a similar Gaussian white noise problem, and akin to the dyadic scheme used in the proof of the KMT approximation by many authors (see, e.g., Komlós, Major, and Tusnády (1975 1976), Mason and van Zwet (1987), Bretagnolle and Massart (1989), Einmahl (1989), Zaitsev (1998), Major (2000), Dudley (2005)). We believe that the main result here (Theorem 1) could lead to a significant simplification of the proof of (Zhou 2004, Theorem 2.1), in analogy with the removal of the inductive part of the proof for the Le Cam distance upper bound between multinomial and multivariate normal experiments from (Carter 2002, Theorem 1), shown in Ouimet (2021). This point is left open for future research.

The general reason that we are interested in developing normal approximations for the Dirichlet density, other than for the two applications given in Section 3 and the potential simplification of the proof of the asymptotic equivalence mentioned above, is because the (multivariate) normal distribution is at the heart of the asymptotic theory for many statistical methods. Any problem that would involve the Dirichlet density and/or its moments (assuming large parameters α and β) can be "transferred", using Theorem 1, to a problem involving the corresponding Gaussian density and/or its moments, which is often easier to deal with. A typical example of this are quantile coupling inequalities (which are ubiquitous in asymptotic theory), where cumulative distribution functions (integrated densities in the continuous setting) need to be compared. Another example could be the derivation optimal Berry-Esseen type bounds, see, e.g., Hipp and Mattner (2007), Dinev and Mattner (2013) and Mattner and Schulz (2018), and references therein. For a general treatment of normal approximations and further motivation on this subject, we refer the reader to Bhattacharya and Ranga Rao (1976), Kolassa (1994) and Chen, Goldstein, and Shao (2011).

Remark 1. Throughout the paper, the notation $u = \mathcal{O}(v)$ means that $\limsup_{N \rightarrow \infty} |u/v| < C$, where $C > 0$ is a universal constant. Whenever C might depend on some parameters, we add subscripts (for example, $u = \mathcal{O}_{\alpha, \beta}(v)$). Also, we write

$$x_{d+1} := 1 - \|x\|_1, \quad \alpha_{d+1} := \beta, \quad \text{and} \quad \varepsilon_N := \frac{1}{N(\|\alpha\|_1 + \beta)}. \quad (7)$$

In particular, the definition of x_{d+1} and r_{d+1} implies that $\delta_{d+1, x_{d+1}} = -\sum_{i=1}^d \delta_{i, x_i}$.

2 | MAIN RESULT

First, we prove an asymptotic expansion for the ratio of the Dirichlet density to the multivariate normal density with the same mean and covariances.

Theorem 1. Pick any $\eta \in (0, 1)$, and let

$$B_\eta := \left\{ x \in \mathcal{S}_d : |\delta_{i, x_i}| \leq \eta N^{1/6}, \text{ for all } i \in \{1, 2, \dots, d+1\} \right\} \quad (8)$$

denote the bulk of the Dirichlet distribution. Then, uniformly for $x \in B_\eta$, we have, as $N \rightarrow \infty$,

$$\begin{aligned} \log \left(\frac{K_{N, \alpha, \beta}(x)}{(1 + \varepsilon_N^{-1})^{d/2} \phi_{\Sigma_r}(\delta_x)} \right) &= \varepsilon_N^{1/2} \cdot \left\{ -\sum_{i=1}^{d+1} \left(\frac{\delta_{i, x_i}}{r_i} \right) + \frac{1}{3} \sum_{i=1}^{d+1} \delta_{i, x_i} \left(\frac{\delta_{i, x_i}}{r_i} \right)^2 \right\} \\ &+ \varepsilon_N \cdot \left\{ \frac{1}{2} \sum_{i=1}^{d+1} (1 + r_i) \left(\frac{\delta_{i, x_i}}{r_i} \right)^2 - \frac{1}{4} \sum_{i=1}^{d+1} \delta_{i, x_i} \left(\frac{\delta_{i, x_i}}{r_i} \right)^3 - \frac{d}{2} + \frac{1}{12} \left\{ 1 - \sum_{i=1}^{d+1} r_i^{-1} \right\} \right\} + \mathcal{O}_{\alpha, \beta, \eta} \left(\frac{(1 + \|\delta_x\|_1)^5}{N^{3/2}} \right). \end{aligned} \quad (9)$$

Some numerical evidence for the validity of this theorem is shown in Appendix B.

Proof of Theorem 1. Using Stirling's formula,

$$\log \Gamma(z) = \frac{1}{2} \log(2\pi) + (z - \frac{1}{2}) \log z - z + \frac{1}{12z} + \mathcal{O}(z^{-3}), \quad z \rightarrow \infty, \quad (10)$$

see, e.g., (Abramowitz & Stegun 1964, p.257), and taking the logarithm in (2), we obtain

$$\begin{aligned} \log K_{N,\alpha,\beta}(\mathbf{x}) &= \log \Gamma(N\|\alpha\|_1 + N\beta) - \sum_{i=1}^{d+1} \log \Gamma(N\alpha_i) + \sum_{i=1}^{d+1} (N\alpha_i - 1) \log x_i \\ &= -\frac{d}{2} \log(2\pi) - \frac{d}{2} \log \varepsilon_N - \frac{1}{2} \sum_{i=1}^{d+1} \log r_i + \sum_{i=1}^{d+1} (N\alpha_i - 1) \log \left(\frac{x_i}{r_i} \right) + \frac{\left\{ 1 - \sum_{i=1}^{d+1} r_i^{-1} \right\}}{12N(\|\alpha\|_1 + \beta)} + \mathcal{O}_{\alpha,\beta}(N^{-3}). \end{aligned} \quad (11)$$

By writing $\frac{x_i}{r_i} = 1 + \frac{\delta_{i,x_i}}{r_i} (1 + \varepsilon_N^{-1})^{-1/2}$ in (11), we deduce

$$\begin{aligned} \log K_{N,\alpha,\beta}(\mathbf{x}) &= -\log \sqrt{(2\pi)^d (1 + \varepsilon_N^{-1})^{-d} \prod_{i=1}^{d+1} r_i} - \frac{d}{2} \log(1 + \varepsilon_N) \\ &\quad + \sum_{i=1}^{d+1} (\varepsilon_N^{-1} r_i - 1) \log \left(1 + \frac{\delta_{i,x_i}}{r_i} (1 + \varepsilon_N^{-1})^{-1/2} \right) + \varepsilon_N \cdot \frac{1}{12} \left\{ 1 - \sum_{i=1}^{d+1} r_i^{-1} \right\} + \mathcal{O}_{\alpha,\beta}(N^{-3}). \end{aligned} \quad (12)$$

By applying the Taylor expansion

$$\log(1 + y) = y - \frac{y^2}{2} + \frac{y^3}{3} - \frac{y^4}{4} + \mathcal{O}_\eta(y^5), \quad \text{valid for } |y| \leq \eta < 1, \quad (13)$$

and noticing that $\delta_{d+1,x_{d+1}} = -\sum_{i=1}^d \delta_{i,x_i}$, we have

$$\begin{aligned} \log K_{N,\alpha,\beta}(\mathbf{x}) &= -\log \sqrt{(2\pi)^d (1 + \varepsilon_N^{-1})^{-d} \prod_{i=1}^{d+1} r_i} - \frac{d}{2} \left\{ \varepsilon_N + \mathcal{O}_{\alpha,\beta}(N^{-2}) \right\} - (1 + \varepsilon_N^{-1})^{-1/2} \sum_{i=1}^{d+1} \frac{\delta_{i,x_i}}{r_i} + \frac{(1 + \varepsilon_N^{-1})^{-1}}{2} \sum_{i=1}^{d+1} \frac{\delta_{i,x_i}^2}{r_i^2} \\ &\quad - (1 + \varepsilon_N)^{-1} \sum_{i=1}^d \frac{\delta_{i,x_i}^2}{2} \left\{ \frac{1}{r_i} - \frac{2}{3} \cdot \frac{\delta_{i,x_i}}{r_i^2} (1 + \varepsilon_N^{-1})^{-1/2} + \frac{1}{2} \cdot \frac{\delta_{i,x_i}^2}{r_i^3} (1 + \varepsilon_N^{-1})^{-1} + \mathcal{O}_{\alpha,\beta,\eta} \left(\frac{(1 + \|\delta_{\mathbf{x}}\|_1)^3}{N^{3/2}} \right) \right\} \\ &\quad - (1 + \varepsilon_N)^{-1} \sum_{i,j=1}^d \frac{\delta_{i,x_i} \delta_{j,x_j}}{2} \left\{ \frac{1}{r_{d+1}} + \frac{2}{3} \cdot \sum_{\ell=1}^d \frac{\delta_{\ell,x_\ell}}{r_{d+1}^2} (1 + \varepsilon_N^{-1})^{-1/2} + \frac{1}{2} \cdot \sum_{\ell,m=1}^d \frac{\delta_{\ell,x_\ell} \delta_{m,x_m}}{r_{d+1}^3} (1 + \varepsilon_N^{-1})^{-1} + \mathcal{O}_{\alpha,\beta,\eta} \left(\frac{(1 + \|\delta_{\mathbf{x}}\|_1)^3}{N^{3/2}} \right) \right\} \\ &\quad + \varepsilon_N \cdot \frac{1}{12} \left\{ 1 - \sum_{i=1}^{d+1} r_i^{-1} \right\} + \mathcal{O}_{\alpha,\beta}(N^{-3}). \end{aligned} \quad (14)$$

We can rewrite this as

$$\begin{aligned} \log K_{N,\alpha,\beta}(\mathbf{x}) &= -\log \sqrt{(2\pi)^d (1 + \varepsilon_N^{-1})^{-d} \prod_{i=1}^{d+1} r_i} - \varepsilon_N^{1/2} \sum_{i=1}^{d+1} \frac{\delta_{i,x_i}}{r_i} + \frac{\varepsilon_N}{2} \sum_{i=1}^{d+1} \frac{\delta_{i,x_i}^2}{r_i^2} - (1 + \varepsilon_N)^{-1} \sum_{i,j=1}^d \frac{\delta_{i,x_i} \delta_{j,x_j}}{2} \{ (\Sigma_r^{-1})_{ij} + S_{N,ij} \} \\ &\quad + \varepsilon_N \cdot \left[-\frac{d}{2} + \frac{1}{12} \left\{ 1 - \sum_{i=1}^{d+1} r_i^{-1} \right\} \right] + \mathcal{O}_{\alpha,\beta,\eta} \left(\frac{(1 + \|\delta_{\mathbf{x}}\|_1)^2}{N^{3/2}} \right). \end{aligned} \quad (15)$$

where the $d \times d$ matrices Σ_r^{-1} and S_N have the (i, j) components:

$$(\Sigma_r^{-1})_{ij} := \frac{1}{r_i} \mathbf{1}_{\{i=j\}} + \frac{1}{r_{d+1}}, \quad (16)$$

$$S_{N,ij} := \frac{2\varepsilon_N^{1/2}}{3} \sum_{\ell=1}^d \frac{\delta_{\ell,x_\ell}}{(1 + \varepsilon_N)^{1/2}} \left\{ \frac{-1}{r_i^2} \mathbf{1}_{\{i=j=\ell\}} + \frac{1}{r_{d+1}^2} \right\} + \frac{\varepsilon_N}{2} \sum_{\ell,m=1}^d \frac{\delta_{\ell,x_\ell} \delta_{m,x_m}}{(1 + \varepsilon_N)} \left\{ \frac{1}{r_i^3} \mathbf{1}_{\{i=j=\ell=m\}} + \frac{1}{r_{d+1}^3} \right\} + \mathcal{O}_{\alpha,\beta,\eta} \left(\frac{(1 + \|\delta_{\mathbf{x}}\|_1)^3}{N^{3/2}} \right). \quad (17)$$

After expanding (18) using $(1 + \varepsilon_N)^{-1} = 1 - \varepsilon_N + \dots$, and rearranging some terms, we get

$$\begin{aligned} \log \left(\frac{K_{N,\alpha,\beta}(\mathbf{x})}{(1 + \varepsilon_N^{-1})^{d/2} \phi_{\Sigma_r}(\delta_{\mathbf{x}})} \right) &= -\varepsilon_N^{1/2} \sum_{i=1}^{d+1} \frac{\delta_{i,x_i}}{r_i} + \frac{\varepsilon_N}{2} \sum_{i=1}^{d+1} \frac{\delta_{i,x_i}^2}{r_i^2} + \varepsilon_N \sum_{i,j=1}^d \frac{\delta_{i,x_i} \delta_{j,x_j}}{2} (\Sigma_r^{-1})_{ij} - \varepsilon_N^{1/2} \sum_{i,j,\ell=1}^d \frac{\delta_{i,x_i} \delta_{j,x_j} \delta_{\ell,x_\ell}}{3} \left\{ \frac{-1}{r_i^2} \mathbf{1}_{\{i=j=\ell\}} + \frac{1}{r_{d+1}^2} \right\} \\ &\quad - \varepsilon_N \sum_{i,j,\ell,m=1}^d \frac{\delta_{i,x_i} \delta_{j,x_j} \delta_{\ell,x_\ell} \delta_{m,x_m}}{4} \left\{ \frac{1}{r_i^3} \mathbf{1}_{\{i=j=\ell=m\}} + \frac{1}{r_{d+1}^3} \right\} + \varepsilon_N \cdot \left[-\frac{d}{2} + \frac{1}{12} \left\{ 1 - \sum_{i=1}^{d+1} r_i^{-1} \right\} \right] \\ &\quad + \mathcal{O}_{\alpha,\beta,\eta} \left(\frac{(1 + \|\delta_{\mathbf{x}}\|_1)^5}{N^{3/2}} \right). \end{aligned} \quad (18)$$

To obtain (9), simply rewrite the above using the fact that $\delta_{d+1,x_{d+1}} = -\sum_{i=1}^d \delta_{i,x_i}$. This ends the proof. $\square$

3 | APPLICATIONS

In this section, we present two applications of Theorem 1. We find an upper bound on the total variation between Dirichlet and multivariate normal distributions (Section 3.1) and we present an alternative proof for the asymptotic variance of Dirichlet kernel estimators found in Theorem 4.2 of Ouimet (2020) (Section 3.2).

3.1 | Total variation bound between Dirichlet and multivariate normal distributions

Theorem 2. Let $(\alpha, \beta) \in (0, \infty)^{d+1}$ be given. Let $\mathbb{P}_{\alpha, \beta}$ be the probability measure on $\mathbb{R}^d$ induced by the Dirichlet($N\alpha, N\beta$) distribution, and let $\mathbb{Q}_{\alpha, \beta}$ be the probability measure on $\mathbb{R}^d$ induced by the Normal $_d(\mathbf{r}, (1 + \varepsilon_N^{-1})^{-1} \Sigma_{\mathbf{r}})$ distribution, where recall $\Sigma_{\mathbf{r}} := \text{diag}(\mathbf{r}) - \mathbf{r}\mathbf{r}^\top$. Then, we have, as $N \rightarrow \infty$,

$$\|\mathbb{P}_{\alpha, \beta} - \mathbb{Q}_{\alpha, \beta}\| = \mathcal{O}\left(\varepsilon_N^{1/2} \cdot d \sqrt{\frac{\max_{1 \leq i \leq d+1} r_i}{\min_{1 \leq i \leq d+1} r_i}}\right), \quad (19)$$

where $\|\cdot\|$ denotes the total variation norm.

Given the many relations there exist between the total variation and other probability metrics such as the discrepancy metric, the Prokhorov metric and the Hellinger distance (see, e.g., (Gibbs & Su 2002, p.421)), many corollaries follow straightforwardly from Theorem 2. The details are omitted for conciseness.

Proof of Theorem 2. Let $\mathbf{X} \sim \mathbb{P}_{\alpha, \beta}$. By the comparison of the total variation norm with the Hellinger distance on page 726 of Carter (2002), we already know that

$$\|\mathbb{P}_{\alpha, \beta} - \mathbb{Q}_{\alpha, \beta}\| \leq \sqrt{2\mathbb{P}(\mathbf{X} \in B_{1/2}^c) + \mathbb{E}\left[\log\left(\frac{d\mathbb{P}_{\alpha, \beta}}{d\mathbb{Q}_{\alpha, \beta}}(\mathbf{X})\right) \mathbb{1}_{\{\mathbf{X} \in B_{1/2}\}}\right]}. \quad (20)$$

Then, by applying a union bound followed by large deviation bounds for the beta distribution (see, e.g., Theorem 2.1 of Marchal and Arbel (2017)), we get, for N large enough,

$$\mathbb{P}(\mathbf{X} \in B_{1/2}^c) \leq \sum_{i=1}^{d+1} \mathbb{P}\left(|\delta_{i, x_i}| > \frac{1}{2} N^{1/6}\right) \leq (d+1) \cdot 2 \exp\left(-\frac{1}{2} N^{1/3}\right). \quad (21)$$

By Theorem 1,

$$\begin{aligned} \mathbb{E}\left[\log\left(\frac{d\mathbb{P}_{\alpha, \beta}}{d\mathbb{Q}_{\alpha, \beta}}(\mathbf{X})\right) \mathbb{1}_{\{\mathbf{X} \in B_{1/2}\}}\right] &= \varepsilon_N^{1/2} \cdot \mathbb{E}\left[\left\{-\sum_{i=1}^d \delta_{i, x_i} \left(\frac{1}{r_i} - \frac{1}{r_{d+1}}\right) + \frac{1}{3} \sum_{i, j, \ell=1}^d \delta_{i, x_i} \delta_{j, x_j} \delta_{\ell, x_\ell} \left(\frac{1}{r_i^2} \mathbb{1}_{\{i=j=\ell\}} - \frac{1}{r_{d+1}^2}\right)\right\} \mathbb{1}_{\{\mathbf{X} \in B_{1/2}\}}\right] \\ &\quad + \varepsilon_N \cdot \mathcal{O}\left(\left|\sum_{i=1}^{d+1} \frac{\mathbb{E}[(X_i - r_i)^2]}{\varepsilon_N r_i^2}\right| + \left|\sum_{i=1}^{d+1} \frac{\mathbb{E}[(X_i - r_i)^4]}{\varepsilon_N^2 r_i^3}\right| + d + \sum_{i=1}^{d+1} r_i^{-1}\right) + \mathcal{O}_{d, \alpha, \beta}(N^{-3/2}). \end{aligned} \quad (22)$$

By Lemma 1, the second to last $\mathcal{O}(\cdot)$ term above is

$$= \mathcal{O}\left(\sum_{i=1}^{d+1} r_i^{-1}\right) = \mathcal{O}\left(\frac{d}{\min_{1 \leq i \leq d+1} r_i}\right) = \mathcal{O}\left(d^2 \frac{\max_{1 \leq i \leq d+1} r_i}{\min_{1 \leq i \leq d+1} r_i}\right). \quad (23)$$

(The last equality follows from $\frac{1}{d+1} \leq \max_{1 \leq i \leq d+1} r_i$, which itself is consequence of the fact that $r_i \geq 0$ and $\sum_{i=1}^{d+1} r_i = 1$.) By putting (23) in (22) and using Lemma 2, we get

$$\begin{aligned} (22) &= \varepsilon_N^{1/2} \cdot \left\{ \frac{\varepsilon_N^2 (1 + \varepsilon_N^{-1})^{3/2}}{3} \cdot \sum_{i, j, \ell=1}^d \frac{\left(4r_i r_j r_\ell - 2r_i r_\ell \mathbb{1}_{\{i=j\}} - 2r_j r_\ell \mathbb{1}_{\{i=\ell\}}\right)}{(1 + \varepsilon_N)(1 + 2\varepsilon_N)} \cdot \left\{\frac{1}{r_i^2} \mathbb{1}_{\{i=j=\ell\}} - \frac{1}{r_{d+1}^2}\right\} + \mathcal{O}\left(\frac{d^3 (\mathbb{P}(\mathbf{X} \in B_{1/2}^c))^{1/4}}{(\min_{1 \leq i \leq d+1} r_i)^2}\right) \right\} \\ &\quad + \varepsilon_N \cdot \mathcal{O}\left(d^2 \frac{\max_{1 \leq i \leq d+1} r_i}{\min_{1 \leq i \leq d+1} r_i}\right) + \mathcal{O}_{d, \alpha, \beta}(N^{-3/2}) \\ &= \mathcal{O}\left(\varepsilon_N^{1/2} \cdot \frac{d^3 (\mathbb{P}(\mathbf{X} \in B_{1/2}^c))^{1/4}}{(\min_{1 \leq i \leq d+1} r_i)^2}\right) + \mathcal{O}\left(\varepsilon_N \cdot d^2 \frac{\max_{1 \leq i \leq d+1} r_i}{\min_{1 \leq i \leq d+1} r_i}\right). \end{aligned} \quad (24)$$

Now, putting (21) and (24) together in (20) gives the conclusion. $\square$

3.2 | Asymptotic variance of Dirichlet kernel estimators

Assume that we have a sequence of observations $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_n$ that are independent and F distributed (F is unknown), with density f supported on the d -dimensional simplex $\mathcal{S}_d$. Then, for a given bandwidth parameter $b > 0$, let

$$\hat{f}_{n,b}(\mathbf{s}) := \frac{1}{n} \sum_{i=1}^n K_{1/b, \mathbf{s}+b, 1-\|\mathbf{s}\|_1+b}(\mathbf{X}_i), \quad \mathbf{s} \in \mathcal{S}_d, \quad (25)$$

be the *Dirichlet kernel estimator* for the density function f . This estimator was introduced by Aitchison and Lauder (1985) as a nonparametric method of density estimation for compositional data and its asymptotic properties were studied theoretically for the first time in Ouimet (2020). For a detailed overview of the literature on asymmetric kernel estimators, we refer the reader to Hirukawa (2018) or Section 2 in Ouimet (2020).

One interesting application of the normal approximation in Theorem 1 is the derivation of the asymptotic variance of $\hat{f}_{n,b}$ at each point $\mathbf{s}$ in the interior of the simplex. This result was already known from Theorem 4.2 in Ouimet (2020), but the method of proof we present here is completely different.

Theorem 3. Assume that f is Lipschitz continuous and let $\mathbf{s} \in \text{Int}(\mathcal{S}_d)$, then

$$\text{Var}(\hat{f}_{n,b}(\mathbf{s})) = \frac{n^{-1}b^{-d/2}(f(\mathbf{s}) + \mathcal{O}_{d,s}(b^{1/2}))}{\sqrt{(4\pi)^d \prod_{i=1}^{d+1} s_i}}, \quad n \rightarrow \infty. \quad (26)$$

From this result, other asymptotic expressions can be derived such as the mean squared error and the mean integrated squared error and we can also optimize the bandwidth parameter b with respect to them, see, e.g., Corollary 4.3 and Theorem 4.4 in Ouimet (2020).

Proof of Theorem 3. Straightforward computations show that

$$\begin{aligned} \text{Var}(\hat{f}_{n,b}(\mathbf{s})) &= n^{-1} \mathbb{E}[K_{1/b, \mathbf{s}+b, 1-\|\mathbf{s}\|_1+b}(\mathbf{X})^2] - n^{-1} \left(\mathbb{E}[K_{1/b, \mathbf{s}+b, 1-\|\mathbf{s}\|_1+b}(\mathbf{X})] \right)^2 \\ &= n^{-1} \mathbb{E}[K_{1/b, \mathbf{s}+b, 1-\|\mathbf{s}\|_1+b}(\mathbf{X})^2] - \mathcal{O}(n^{-1}), \end{aligned} \quad (27)$$

where

$$\begin{aligned} \mathbb{E}[K_{1/b, \mathbf{s}+b, 1-\|\mathbf{s}\|_1+b}(\mathbf{X})^2] &\stackrel{(9)}{=} \int_{\mathcal{S}_d} \left(\frac{\exp\left(-\frac{1}{2} \delta_{\mathbf{x}}^T \Sigma_r^{-1} \delta_{\mathbf{x}}\right)}{\sqrt{(2\pi)^d (1 + \varepsilon_N^{-1})^{-d} \prod_{i=1}^{d+1} r_i}} \right)^2 f(\mathbf{x}) d\mathbf{x} + o_{d,s}(1) \\ &= \frac{2^{-d/2}(f(\mathbf{s}) + \mathcal{O}_{d,s}(b^{1/2}))}{\sqrt{(2\pi)^d b^d \prod_{i=1}^{d+1} r_i}} \int_{\mathcal{S}_d} \frac{\exp\left(-\frac{1}{2} \delta_{\mathbf{x}}^T (\frac{1}{2} \Sigma_r)^{-1} \delta_{\mathbf{x}}\right)}{\sqrt{(2\pi)^d 2^{-d} (1 + \varepsilon_N^{-1})^{-d} \prod_{i=1}^{d+1} r_i}} d\mathbf{x} + o_{d,s}(1) \\ &= \frac{b^{-d/2}(f(\mathbf{s}) + \mathcal{O}_{d,s}(b^{1/2}))}{\sqrt{(4\pi)^d \prod_{i=1}^{d+1} r_i}} (1 + o_d(1)) + o_{d,s}(1). \end{aligned} \quad (28)$$

Since $r_i = (s_i + b)/(1 + b(d+1)) = s_i + o_{d,s}(1)$ for all $i \in \{1, 2, \dots, d+1\}$, plugging the estimate (28) in (27) gives us the conclusion. $\square$

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APPENDIX

A MOMENTS OF THE DIRICHLET DISTRIBUTION

Below, we compute some of the central moments (up to four) of the Dirichlet distribution. The lemma is used to estimate the $\asymp \varepsilon_N$ errors in (22) of the proof of Theorem 2, and also as a preliminary result for the proof of Lemma 2.

Lemma 1. Let $N \in \mathbb{N}$ and $(\alpha, \beta) \in (0, \infty)^{d+1}$ be given. If $\mathbf{X} = (X_1, X_2, \dots, X_d) \sim \text{Dirichlet}(N\alpha, N\beta)$ according to (2), then, for all $i, j, \ell \in \{1, 2, \dots, d\}$,

$$\mathbb{E}[(X_i - r_i)(X_j - r_j)] = \varepsilon_N r_i \cdot \frac{(\mathbb{1}_{\{i=j\}} - r_j)}{(1 + \varepsilon_N)}, \quad (A1)$$

$$\mathbb{E}[(X_i - r_i)(X_j - r_j)(X_\ell - r_\ell)] = \varepsilon_N^2 \cdot \frac{(4r_i r_j r_\ell - 2r_i r_\ell \mathbb{1}_{\{i=j\}} - 2r_j r_\ell \mathbb{1}_{\{i=\ell\}} - 2r_i r_j \mathbb{1}_{\{j=\ell\}} + 2r_i \mathbb{1}_{\{i=j=\ell\}})}{(1 + \varepsilon_N)(1 + 2\varepsilon_N)}, \quad (A2)$$

$$\mathbb{E}[(X_i - r_i)^4] = \varepsilon_N^2 r_i^2 \cdot 3(1 - r_i)^2 + \mathcal{O}_{\alpha, \beta}(N^{-3}), \quad (A3)$$

where recall $\varepsilon_N := 1/(N\|\alpha\|_1 + N\beta)$ and $r_i := \mathbb{E}[X_i] = \alpha_i/(\|\alpha\|_1 + \beta)$ for all $i \in \{1, 2, \dots, d\}$.

Proof of Lemma 1. Equation (A1) can be found in (Ng et al. 2011, p.39). Since

$$\begin{aligned} \mathbb{E}[X_i X_j] &= \begin{cases} \frac{\Gamma(N\alpha_i+1)\Gamma(N\alpha_j+1)}{\Gamma(N\alpha_i)\Gamma(N\alpha_j)} \cdot \frac{\Gamma(N\|\alpha\|_1+N\beta)}{\Gamma(N\|\alpha\|_1+N\beta+2)}, & \text{if } i \neq j, \\ \frac{\Gamma(N\alpha_i+2)}{\Gamma(N\alpha_i)} \cdot \frac{\Gamma(N\|\alpha\|_1+N\beta)}{\Gamma(N\|\alpha\|_1+N\beta+2)}, & \text{if } i = j, \end{cases} \\ &= \frac{\alpha_i(\alpha_j + \mathbb{1}_{\{i=j\}}N^{-1})}{(\|\alpha\|_1 + \beta)(\|\alpha\|_1 + \beta + N^{-1})}, \end{aligned} \quad (\text{A4})$$

and

$$\begin{aligned} \mathbb{E}[X_i X_j X_\ell] &= \begin{cases} \frac{\Gamma(N\alpha_i+1)\Gamma(N\alpha_j+1)\Gamma(N\alpha_\ell+1)}{\Gamma(N\alpha_i)\Gamma(N\alpha_j)\Gamma(N\alpha_\ell)} \cdot \frac{\Gamma(N\|\alpha\|_1+N\beta)}{\Gamma(N\|\alpha\|_1+N\beta+3)}, & \text{if } i \neq j \neq \ell \neq i, \\ \frac{\Gamma(N\alpha_i+2)\Gamma(N\alpha_\ell+1)}{\Gamma(N\alpha_i)\Gamma(N\alpha_\ell)} \cdot \frac{\Gamma(N\|\alpha\|_1+N\beta)}{\Gamma(N\|\alpha\|_1+N\beta+3)}, & \text{if } i = j \neq \ell, \\ \frac{\Gamma(N\alpha_i+2)\Gamma(N\alpha_j+1)}{\Gamma(N\alpha_i)\Gamma(N\alpha_j)} \cdot \frac{\Gamma(N\|\alpha\|_1+N\beta)}{\Gamma(N\|\alpha\|_1+N\beta+3)}, & \text{if } i = \ell \neq j, \\ \frac{\Gamma(N\alpha_i+1)\Gamma(N\alpha_j+2)}{\Gamma(N\alpha_i)\Gamma(N\alpha_j)} \cdot \frac{\Gamma(N\|\alpha\|_1+N\beta)}{\Gamma(N\|\alpha\|_1+N\beta+3)}, & \text{if } j = \ell \neq i, \\ \frac{\Gamma(N\alpha_i+3)}{\Gamma(N\alpha_i)} \cdot \frac{\Gamma(N\|\alpha\|_1+N\beta)}{\Gamma(N\|\alpha\|_1+N\beta+3)}, & \text{if } i = j = \ell, \end{cases} \\ &= \frac{(\alpha_i + \mathbb{1}_{\{i \neq j\}}N^{-1})(\alpha_j + \mathbb{1}_{\{i=j\}}N^{-1})(\alpha_\ell + \mathbb{1}_{\{j=\ell\}}N^{-1} + \mathbb{1}_{\{i=j=\ell\}}N^{-1})}{(\|\alpha\|_1 + \beta)(\|\alpha\|_1 + \beta + N^{-1})(\|\alpha\|_1 + \beta + 2N^{-1})}, \end{aligned} \quad (\text{A5})$$

we have

$$\begin{aligned} \mathbb{E}[(X_i - r_i)(X_j - r_j)(X_\ell - r_\ell)] &= \mathbb{E}[X_i X_j X_\ell] - r_\ell \mathbb{E}[X_i X_j] - r_j \mathbb{E}[X_i X_\ell] - r_i \mathbb{E}[X_j X_\ell] + 2r_i r_j r_\ell \\ &= \frac{\left\{ \begin{aligned} &(\alpha_i + \mathbb{1}_{\{i \neq j\}}N^{-1})(\alpha_j + \mathbb{1}_{\{i=j\}}N^{-1})(\alpha_\ell + (\mathbb{1}_{\{j=\ell\}} + \mathbb{1}_{\{i=j=\ell\}})N^{-1}) \cdot (\|\alpha\|_1 + \beta)^2 \\ &- \alpha_i \alpha_\ell (\alpha_j + \mathbb{1}_{\{i=j\}}N^{-1}) \cdot (\|\alpha\|_1 + \beta)(\|\alpha\|_1 + \beta + 2N^{-1}) \\ &- \alpha_i \alpha_j (\alpha_\ell + \mathbb{1}_{\{i=\ell\}}N^{-1}) \cdot (\|\alpha\|_1 + \beta)(\|\alpha\|_1 + \beta + 2N^{-1}) \\ &- \alpha_i \alpha_j (\alpha_\ell + \mathbb{1}_{\{j=\ell\}}N^{-1}) \cdot (\|\alpha\|_1 + \beta)(\|\alpha\|_1 + \beta + 2N^{-1}) \\ &+ 2\alpha_i \alpha_j \alpha_\ell \cdot (\|\alpha\|_1 + \beta + N^{-1})(\|\alpha\|_1 + \beta + 2N^{-1}) \end{aligned} \right\}}{(\|\alpha\|_1 + \beta)^3(\|\alpha\|_1 + \beta + N^{-1})(\|\alpha\|_1 + \beta + 2N^{-1})} \\ &= N^{-2} \cdot \frac{\left\{ \begin{aligned} &4\alpha_i \alpha_j \alpha_\ell - 2\alpha_i \alpha_\ell \mathbb{1}_{\{i=j\}}(\|\alpha\|_1 + \beta) - 2\alpha_j \alpha_\ell \mathbb{1}_{\{i=\ell\}}(\|\alpha\|_1 + \beta) \\ &- 2\alpha_i \alpha_j \mathbb{1}_{\{j=\ell\}}(\|\alpha\|_1 + \beta) + 2\alpha_i \mathbb{1}_{\{i=j=\ell\}}(\|\alpha\|_1 + \beta)^2 \end{aligned} \right\}}{(\|\alpha\|_1 + \beta)^3(\|\alpha\|_1 + \beta + N^{-1})(\|\alpha\|_1 + \beta + 2N^{-1})} \\ &= N^{-2} \cdot \frac{(4r_i r_j r_\ell - 2r_i r_\ell \mathbb{1}_{\{i=j\}} - 2r_j r_\ell \mathbb{1}_{\{i=\ell\}} - 2r_i r_j \mathbb{1}_{\{j=\ell\}} + 2r_i \mathbb{1}_{\{i=j=\ell\}})}{(\|\alpha\|_1 + \beta + N^{-1})(\|\alpha\|_1 + \beta + 2N^{-1})}, \end{aligned} \quad (\text{A6})$$

which proves (A2). Finally, trivial calculations show that

$$\begin{aligned} \mathbb{E}[X_i^4] &= \frac{\Gamma(N\alpha_i+4)}{\Gamma(N\alpha_i)} \cdot \frac{\Gamma(N\|\alpha\|_1+N\beta)}{\Gamma(N\|\alpha\|_1+N\beta+4)} \\ &= \frac{N\alpha_i(N\alpha_i+1)(N\alpha_i+2)(N\alpha_i+3) \cdot N^3(\|\alpha\|_1 + \beta)^3}{N^7(\|\alpha\|_1 + \beta)^7 \cdot (1 + \mathcal{O}_{\alpha,\beta}(N^{-1}))}. \end{aligned} \quad (\text{A7})$$

We deduce

$$\begin{aligned} \mathbb{E}[(X_i - r_i)^4] &= \mathbb{E}[X_i^4] - 4r_i \mathbb{E}[X_i^3] + 6r_i^2 \mathbb{E}[X_i^2] - 3r_i^4 \\ &= \frac{\left\{ \begin{aligned} &N\alpha_i(N\alpha_i+1)(N\alpha_i+2)(N\alpha_i+3) \cdot N^3(\|\alpha\|_1 + \beta)^3 \\ &- 4N^2\alpha_i^2(N\alpha_i+1)(N\alpha_i+2) \cdot N^2(\|\alpha\|_1 + \beta)^2(N\|\alpha\|_1 + N\beta + 3) \\ &+ 6N^3\alpha_i^3(N\alpha_i+1) \cdot N(\|\alpha\|_1 + \beta) \prod_{\ell=2}^3(N\|\alpha\|_1 + N\beta + \ell) \\ &- 3N^4\alpha_i^4 \cdot \prod_{\ell=1}^3(N\|\alpha\|_1 + N\beta + \ell) \end{aligned} \right\}}{N^7(\|\alpha\|_1 + \beta)^7 \cdot (1 + \mathcal{O}_{\alpha,\beta}(N^{-1}))} \\ &= N^{-2} \cdot \frac{3\alpha_i^2(\|\alpha\|_1 - \alpha_i + \beta)^2}{(\|\alpha\|_1 + \beta)^6} + \mathcal{O}_{\alpha,\beta}(N^{-3}), \end{aligned} \quad (\text{A8})$$

which proves (A3). This ends the proof. $\square$

We can also estimate the moments of Lemma 1 on various events. The lemma below is used to estimate the $\asymp \varepsilon_N^{1/2}$ errors in (22) of the proof of Theorem 2.

Lemma 2. Let $(\alpha, \beta) \in (0, \infty)^{d+1}$ be given, and let $A \in \mathcal{B}(\mathbb{R}^d)$ be a Borel set. If $\mathbf{X} = (X_1, X_2, \dots, X_d) \sim \text{Dirichlet}(N\alpha, N\beta)$ according to (2), then, for all $i, j, \ell \in \{1, 2, \dots, d\}$ and N large enough,

$$\left| \mathbb{E}[(X_i - r_i) \mathbb{1}_{\{\mathbf{X} \in A\}}] \right| \leq \varepsilon_N^{1/2} (\mathbb{P}(\mathbf{X} \in A^c))^{1/2}, \quad (\text{A9})$$

$$\left| \mathbb{E}[(X_i - r_i)(X_j - r_j)(X_\ell - r_\ell) \mathbb{1}_{\{\mathbf{X} \in A\}}] - \varepsilon_N^2 \cdot \frac{(4r_i r_j r_\ell - 2r_i r_\ell \mathbb{1}_{\{i=j\}} - 2r_j r_\ell \mathbb{1}_{\{i=\ell\}} - 2r_i r_j \mathbb{1}_{\{j=\ell\}} + 2r_i \mathbb{1}_{\{i=j=\ell\}})}{(1 + \varepsilon_N)(1 + 2\varepsilon_N)} \right| \leq \varepsilon_N^{3/2} (\mathbb{P}(\mathbf{X} \in A^c))^{1/4}, \quad (\text{A10})$$

where recall $\varepsilon_N := 1/(N\|\alpha\|_1 + N\beta)$ and $r_i := \mathbb{E}[X_i] = \alpha_i/(\|\alpha\|_1 + \beta)$ for all $i \in \{1, 2, \dots, d\}$.

Proof of Lemma 2. For the bound in (A9), note that $\mathbb{E}[X_i - r_i] = 0$. By Cauchy-Schwarz and a bound on the second moment of the beta distribution (see, e.g., (A1)), we have

$$\left| \mathbb{E}[(X_i - r_i) \mathbb{1}_{\{\mathbf{X} \in A\}}] \right| = \left| \mathbb{E}[(X_i - r_i) \mathbb{1}_{\{\mathbf{X} \in A^c\}}] \right| \leq \left(\mathbb{E}[(X_i - r_i)^2] \right)^{1/2} (\mathbb{P}(\mathbf{X} \in A^c))^{1/2} \leq \varepsilon_N^{1/2} (\mathbb{P}(\mathbf{X} \in A^c))^{1/2}. \quad (\text{A11})$$

For the bound in (A10), Equation (A2), Hölder's inequality and a bound on the fourth central moment of the beta distribution (see, e.g., (A3)) yield, for N large enough,

$$\begin{aligned} & \left| \mathbb{E}[(X_i - r_i)(X_j - r_j)(X_\ell - r_\ell) \mathbb{1}_{\{\mathbf{X} \in A\}}] - \varepsilon_N^2 \cdot \frac{(4r_i r_j r_\ell - 2r_i r_\ell \mathbb{1}_{\{i=j\}} - 2r_j r_\ell \mathbb{1}_{\{i=\ell\}} - 2r_i r_j \mathbb{1}_{\{j=\ell\}} + 2r_i \mathbb{1}_{\{i=j=\ell\}})}{(1 + \varepsilon_N)(1 + 2\varepsilon_N)} \right| \\ &= \left| \mathbb{E}[(X_i - r_i)(X_j - r_j)(X_\ell - r_\ell) \mathbb{1}_{\{\mathbf{X} \in A^c\}}] \right| \\ &\leq \left(\mathbb{E}[(X_i - r_i)^4] \right)^{1/4} \left(\mathbb{E}[(X_j - r_j)^4] \right)^{1/4} \left(\mathbb{E}[(X_\ell - r_\ell)^4] \right)^{1/4} (\mathbb{P}(\mathbf{X} \in A^c))^{1/4} \\ &\leq \varepsilon_N^{1/2} \varepsilon_N^{1/2} \varepsilon_N^{1/2} (\mathbb{P}(\mathbf{X} \in A^c))^{1/4}. \end{aligned} \quad (\text{A12})$$

This ends the proof. $\square$

B SIMULATIONS

In this appendix, we provide some numerical evidence (displayed graphically) for the validity of the expansion in Theorem 1. We compare three levels of approximation for various choices of α and β . For any given $(\alpha, \beta) \in (0, \infty)^{d+1}$, define

$$E_0 := \sup_{\mathbf{x} \in \mathbb{R}^d: \|\mathbf{x} - \mathbf{r}\|_\infty \leq \varepsilon_N^{1/2}} \left| \log \left(\frac{K_{N, \alpha, \beta}(\mathbf{x})}{(1 + \varepsilon_N^{-1})^{d/2} \phi_{\Sigma_r}(\delta_{\mathbf{x}})} \right) \right|, \quad (\text{B13})$$

$$E_1 := \sup_{\mathbf{x} \in \mathbb{R}^d: \|\mathbf{x} - \mathbf{r}\|_\infty \leq \varepsilon_N^{1/2}} \left| \log \left(\frac{K_{N, \alpha, \beta}(\mathbf{x})}{(1 + \varepsilon_N^{-1})^{d/2} \phi_{\Sigma_r}(\delta_{\mathbf{x}})} \right) - \varepsilon_N^{1/2} \cdot \left\{ - \sum_{i=1}^{d+1} \left(\frac{\delta_{i, x_i}}{r_i} \right) + \frac{1}{3} \sum_{i=1}^{d+1} \delta_{i, x_i} \left(\frac{\delta_{i, x_i}}{r_i} \right)^2 \right\} \right|, \quad (\text{B14})$$

$$\begin{aligned} E_2 := \sup_{\mathbf{x} \in \mathbb{R}^d: \|\mathbf{x} - \mathbf{r}\|_\infty \leq \varepsilon_N^{1/2}} & \left| \log \left(\frac{K_{N, \alpha, \beta}(\mathbf{x})}{(1 + \varepsilon_N^{-1})^{d/2} \phi_{\Sigma_r}(\delta_{\mathbf{x}})} \right) - \varepsilon_N^{1/2} \cdot \left\{ - \sum_{i=1}^{d+1} \left(\frac{\delta_{i, x_i}}{r_i} \right) + \frac{1}{3} \sum_{i=1}^{d+1} \delta_{i, x_i} \left(\frac{\delta_{i, x_i}}{r_i} \right)^2 \right\} \right. \\ & \left. - \varepsilon_N \cdot \left\{ \frac{1}{2} \sum_{i=1}^{d+1} (1 + r_i) \left(\frac{\delta_{i, x_i}}{r_i} \right)^2 - \frac{1}{4} \sum_{i=1}^{d+1} \delta_{i, x_i} \left(\frac{\delta_{i, x_i}}{r_i} \right)^3 - \frac{d}{2} + \frac{1}{12} \left\{ 1 - \sum_{i=1}^{d+1} r_i^{-1} \right\} \right\} \right|. \end{aligned} \quad (\text{B15})$$

Note that $\|\mathbf{x} - \mathbf{r}\|_\infty \leq \varepsilon_N^{1/2}$ implies $\|\delta_{\mathbf{x}}\|_\infty \leq (1 + \varepsilon_N)^{1/2} \approx 1$, so we expect from Theorem 1 that the errors above (E_0 , E_1 and E_2) will have the asymptotic behavior

$$E_i = \mathcal{O}_{d, \alpha, \beta}(\varepsilon_N^{(1+i)/2}), \quad \text{for all } i \in \{0, 1, 2\}, \quad (\text{B16})$$

or equivalently,

$$\liminf_{N \rightarrow \infty} \frac{\log E_i}{\log \varepsilon_N} \geq \frac{1+i}{2}, \quad \text{for all } i \in \{0, 1, 2\}. \quad (\text{B17})$$

The property (B17) is illustrated in Figures B2, B4 and B6 below, for various choices of α and β . Similarly, the corresponding log-log plots of the errors as a function of N are displayed in Figures B1, B3 and B5. The simulations are limited to $N \leq 10^5$ because numerical errors start to perturb the results near that point, but the evidence remains overwhelming.

FIGURE B1 Plots of $1/E_i$ as a function of N , for various choices of α , when $\beta = 1$. Both the horizontal and vertical axes are on a logarithmic scale. The plots clearly illustrate how the addition of correction terms from Theorem 1 to the base approximation (B13) improves it.

FIGURE B2 Plots of $\log E_i / \log \epsilon_N$ as a function of N , for various choices of α , when $\beta = 1$. The horizontal axis is on a logarithmic scale. The plots confirm (B17) and bring strong evidence for the validity of Theorem 1.

FIGURE B3 Plots of $1/E_i$ as a function of N , for various choices of α , when $\beta = 2$. Both the horizontal and vertical axes are on a logarithmic scale. The plots clearly illustrate how the addition of correction terms from Theorem 1 to the base approximation (B13) improves it.

FIGURE B4 Plots of $\log E_i / \log \epsilon_N$ as a function of N , for various choices of α , when $\beta = 2$. The horizontal axis is on a logarithmic scale. The plots confirm (B17) and bring strong evidence for the validity of Theorem 1.

FIGURE B5 Plots of $1/E_i$ as a function of N , for various choices of α , when $\beta = 3$. Both the horizontal and vertical axes are on a logarithmic scale. The plots clearly illustrate how the addition of correction terms from Theorem 1 to the base approximation (B13) improves it.

FIGURE B6 Plots of $\log E_i / \log \epsilon_N$ as a function of N , for various choices of α , when $\beta = 3$. The horizontal axis is on a logarithmic scale. The plots confirm (B17) and bring strong evidence for the validity of Theorem 1.

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DATA AVAILABILITY STATEMENT

The R code that generated all the figures in Appendix B is available as supplemental material online.

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