Asymptotic properties of Dirichlet kernel density estimators

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Abstract

We study theoretically, for the first time, the Dirichlet kernel estimator introduced by Aitchison and Lauder [3] for the estimation of multivariate densities supported on the $d$-dimensional simplex. The simplex is an important case as it is the natural domain of compositional data and has been neglected in the literature on asymmetric kernels. The Dirichlet kernel estimator, which generalizes the (non-modified) unidimensional Beta kernel estimator from Chen [34], is free of boundary bias and non-negative everywhere on the simplex. We show that it achieves the optimal convergence rate $O(n^{-4/(d+4)})$ for the mean squared error and the mean integrated squared error, we prove its asymptotic normality and uniform strong consistency, and we also find an asymptotic expression for the mean integrated absolute error. To illustrate the Dirichlet kernel method and its favorable boundary properties, we present a case study on minerals processing.

Keywords: Dirichlet kernel, Beta kernel, asymmetric kernel, density estimation, simplex, boundary bias, variance, mean squared error, mean integrated absolute error, asymptotic normality, strong consistency, multivariate associated kernels

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1. Introduction

Kernel smoothing or kernel density estimation is a well-known methodology to characterize (and visualize) the probability density function of a random variable or random vector in a nonparametric way. It can be considered as a bin-free alternative to histograms, and is particularly useful in multivariate cases with a low to moderate number of dimensions, where the accuracy of histograms dramatically deteriorates with the number of variables due to the curse of dimensionality. Apart from visualization purposes, density estimation can be used for nonparametric alternatives to regression and classification (both supervised and unsupervised). One of the most intuitive usages, for instance, is to construct conditional density plots (in R command “cdplot”), to represent how the conditional probabilities of a categorical variable depends on quantitative covariables. This is true in particular for compositional data, but methods of density estimation on the simplex that address the well-known spillover problem of traditional kernel estimators are very scarce in the literature, and theoretical results specific to the simplex are almost nonexistent. To remedy this situation, our main goal in this paper is to revisit the Dirichlet kernel estimator on the simplex introduced by Aitchison and Lauder [3] and study its asymptotic properties in details. A case study on minerals processing presented in Section 5 will show an explicit and elaborate use of conditional density plots using Dirichlet kernel estimators.

Nevertheless, our main contribution in this paper remains theoretical. We will find asymptotic expressions for the pointwise bias, the pointwise variance, the mean squared error (MSE) and the mean integrated squared error (MISE). These results generalize the ones for the Beta kernel in [34] ($d = 1$). The optimal bandwidth parameters $b$, with respect to MSE and MISE, are also written explicitly. In practice, this can be used to implement a plug-in selection method for the bandwidth parameter. The asymptotic normality follows from a straightforward verification of the Lindeberg condition for double arrays, although it is completely new even for Beta kernel estimators. We also obtain the asymptotics of the mean integrated absolute error (MIAE) and the uniform strong consistency, which generalize the results from Bouezmarni and Rolin [16]. To be more precise, the proof of the $L^1$ asymptotics follows the same strategy but the proof of the uniform strong consistency is completely different and represents our biggest contribution (we combine estimates on the difference of Dirichlet densities with different parameters together with a novel chaining argument). Our rates of convergence for the MSE and MISE are optimal, as they coincide (assuming the identification $b \approx b^2$) with the rates of convergence for the MSE and MISE of traditional multivariate kernel estimators, studied for example in [148]. In contrast to other methods of boundary bias reduction (such as the reflection method or boundary kernels (see, e.g., [156])), this property
is built-in for Dirichlet kernel estimators, which makes them one of the easiest to use in the class of estimators that are asymptotically unbiased near (and on) the boundary. Dirichlet kernel estimators are also non-negative everywhere on their domain, which is definitely not the case of many estimators corrected for boundary bias. This is another reason for their desirability. Bandwidth selection methods and their consistency will be investigated thoroughly in upcoming work.

Here is the outline of the paper. In Section 2, we present an overview of the literature of asymmetric kernels. In Section 3, we define Dirichlet kernel estimators, we state some of their basic properties, and we show that Dirichlet kernels are continuous examples in the broader class of multivariate associated kernels introduced by Kokonendji and Somé [111, 112]. In Section 4, our main results are stated, which consists of the asymptotic behavior of the pointwise bias and variance (including points near the boundary of the simplex), the mean squared error, the integrated mean squared error, the mean integrated absolute error, the uniform consistency and the asymptotic normality. All the proofs are gathered in Section 6. In Section 5, the case study on minerals processing is presented.

2. Overview of the literature

Below, we give a systematic overview of the main line of articles on density estimation using Beta kernels (i.e., Dirichlet kernels with \( d = 1 \)), and then we briefly mention several other classes of asymmetric kernels with references. There might be more details than the reader expects, but this is because the subject is vast and relatively important references are often disjointed or missing in the literature, which makes it hard for newcomers to get a complete chronological account of the progress in the field.

Aitchison and Lauder [3] were the first to define the Dirichlet kernel estimator from (2) for the purpose of density estimation. The paper compared their performance empirically with an alternative approach, called the logistic-normal kernel method, where the data on the simplex is first sent to \( \mathbb{R}^d \) via an additive log-ratio transformation and a multivariate Gaussian kernel smoothing is applied afterwards. The authors recommended Dirichlet kernels over the logistic-normal kernel method if there was a suspicion of sparseness in the data. To the best of our knowledge, Chacón et al. [25] were, until now, the only other authors to mention Dirichlet kernels, or even kernel smoothing on the simplex, in any meaningful way. They compared numerically the outcome of different ways of establishing the bandwidth covariance structure of an additive logistic normal kernel: a full bandwidth matrix chosen by cross-validation, a full bandwidth matrix chosen by unconstrained plug-in method, and the logistic-normal kernel method presented in [3] with a bandwidth matrix \( H = hS \) (\( S \) is the sample covariance matrix and \( h \) is chosen to maximize the pseudo-likelihood).

Brown and Chen [24] were the first to study Beta kernels (\( d = 1 \)) theoretically, and they did so in the context of smoothing for regression curves with equally spaced and fixed design points. The asymptotics of the pointwise bias, the integrated variance and the MISE for the estimator of the regression function were found (the optimal MISE was shown to be \( O(n^{-4/5}) \)). These results extended to Beta kernel estimators some parts of the results from Stadtmüller [166], who was working with the closely related Bernstein estimators. Chen [34] was the first author to study (unmodified) Beta kernel estimators (\( \hat{f}_1 \)) theoretically in the context of density estimation. A certain boundary Beta kernel modification, denoted by \( \hat{f}_2 \), was also considered. The asymptotics of the pointwise bias, pointwise variance of both \( \hat{f}_1 \) and \( \hat{f}_2 \) were found everywhere on \([0, 1]\) as well as the MISE (the optimal MISE was shown to be \( O(n^{-4/5}) \)). Numerical comparisons of the estimators were made with the local linear estimator of Lejeune and Sarda [120] and Jones [97] and the non-negative modification proposed by Jones and Foster [99], although various criticisms were raised by Zhang and Karunamuni [185]. Chen [35] generalized the results of Brown and Chen [24] to arbitrary collections of fixed design points using a Gasser-Müller type estimator (Gasser and Müller [55]). A boundary Beta kernel modification, analogous to \( \hat{f}_2 \) from Chen [34], was also considered and the asymptotic results were also extended to that regression curve estimator. In [37], those results were further extended to stochastic design points using a local linear smoother with Beta kernel (and Gamma kernel when the data is supported on \([0, \infty)\) instead of \([0, 1]\)) analogous to the traditional version proposed by Fan and Gijbels [46].

Bouezmarni and Rolin [16] computed the asymptotics of the MIAE for Beta kernel estimators, which extended the analogous result for traditional kernel estimators found in Theorem 2 of Devroye and Penrod [40]. As pointed out by Scott [156, p.44], there are many reasons to estimate the MIAE as it enjoys many advantages over the MISE. It puts more emphasis on the tails of the target density, it is a dimensionless quantity, it is invariant to monotone changes of scale, and it is uniformly bounded (by 2). (For a thorough study of the \( L^1 \) point of view, see Devroye and Györfi [39].) Another result that was proved by Bouezmarni and Rolin [16] for Beta kernel estimators is the uniform strong consistency, which extended the analogous result for traditional kernel estimators found in Theorem 1 of Devroye and Penrod [41]. However, the proof in [16] is completely different. They apply an integration by parts trick to relate \( \sup_{x \in [0,1]} |\hat{f}_{\text{dirichlet}}(x) - \mathbb{E}[\hat{f}_{\text{dirichlet}}(x)]| \) to the supremum of the recentered empirical c.d.f. and then estimate the latter with the Dvoretzky-Kiefer-Wolfowitz inequality. In the context of Bernstein estimators (see, e.g., Babu et al. [4]), a similar idea (its discrete version) was to apply a union bound on a partition of the support of the target density into small boxes and then use concentration bounds on the supremum of "increments" of the recentered empirical c.d.f. inside each box, where the width of the boxes
is carefully chosen so that the bounds are summable and the result follows by the Borel-Cantelli lemma. In the present paper, we will instead apply a novel chaining argument (that might be of independent interest) and give ourselves a buffer on the boundary to avoid technical issues related to the partial derivatives of the Dirichlet density \( K_{\alpha,\beta} \) with respect to \( \alpha_1, \ldots, \alpha_d, \beta \). It is not obvious how to generalize the proof of Bouezmarni and Rolin [16] on the simplex.

Renault and Scaillet [149] were the first to use Beta kernels to estimate recovery rate densities of defaulted bonds. They also investigated the finite sample performance of the Beta kernel density estimator by comparing the averages of integrated squared errors of Monte Carlo samples against two other methods: traditional Gaussian kernel smoothing, and a logistic transformation combined with traditional Gaussian kernel smoothing and a back transformation of the estimated density by multiplying it with the derivative of the inverse mapping (i.e., the appropriate Jacobian). Furthermore, they showed that the usual practice of approximating the recovery function through a Beta density calibrated with the sample mean and variance should be handled with caution as the inflexibility of the parametric approach can lead (for example) to an underestimated of the Value-at-Risk. Gouriéroux and Monfort [63] showed the non-consistency of the Beta kernel approach to estimate the recovery rate density when there are point masses at 0 (total loss) or 1 (total recovery). Without point masses at 0 or 1, the Beta kernel approach features significant bias in finite sample according to the authors. In large sample, the method is consistent, but they showed that competing approaches (called micro-Beta and macro-Beta; these are two types of normalization of the vanilla Beta kernel estimator) can provide more accurate results when estimating the continuous part of the loss-given-default distribution.

Fernandes and Monteiro [51] derived the asymptotic behavior of Beta kernel functionals (and Gamma kernel functionals when the support of the target density \( f \) is \([0, \infty)\) instead of \([0, 1]\)) of the form

\[
\int_A \varphi(x)(f_{\alpha,\beta}(x) - f(x))dx,
\]

where \( \varphi \) is a bounded regular function and \( A \) is the support of \( f \), by applying a central limit theorem for degenerate \( U \)-statistics with variable kernel. The ideas are similar to those applied by Hall [66] for traditional kernel estimators.

Hirukawa [73] applied two multiplicative bias correction methods (from Terrell and Scott [172] and Jones et al. [101], respectively) to the two Beta kernel estimators from Chen [34], which, under sufficient smoothness conditions on the target density, had an effect of reducing the pointwise bias while the order of magnitude of the pointwise variance stayed the same. Under the assumption that the target density is four-times continuously differentiable, the asymptotics of the pointwise bias, pointwise variance, MSE and MISE were found (the optimal rate of convergence was also shown to be \( O(n^{-8/9}) \) for the MISE and MSE inside \((0, 1)\), instead of the usual \( O(n^{-4/5}) \)). Hirukawa also investigated the numerical performance of the Beta and modified Beta kernel estimators of Chen [34] as well as them under the micro/macro normalizations from Gouriéroux and Monfort [63], and all these combinations (except for micro) under the two aforementioned multiplicative bias correction methods. For all 14 combinations that were studied, the bandwidth parameter was selected according to two methods: rule-of-thumb and plug-in. He concluded that the estimators corrected for bias under the JLN-method of Jones et al. [101] had a superior performance compared to the bias-uncorrected estimators.

Bouezmarni and Rombouts [20] generalized the results of Chen [34, 36] to the multidimensional setting. The kernels that they considered were the products of one-dimensional asymmetric kernels (Beta kernels, modified Beta kernels, or Gamma kernels, modified Gamma kernels, local linear kernel; depending on the support of the marginals of the target density). Asymptotics of the pointwise bias, pointwise variance and MISE were found. The authors also proved the asymptotic normality, uniform strong consistency and the almost-sure convergence of the MISE when the bandwidth parameter \( b \) is selected via a least-square cross-validation method. The finite sample performance of the estimators were investigated by comparing the mean and standard deviation of integrated squared errors of Monte Carlo samples under various target densities. When the target density is supported on \([0, \infty)\), their results showed that the proposed estimators perform almost as well as the traditional Gaussian kernel estimator when there are no boundary problems, and in general, the modified Gamma and local linear estimators dominate the other estimators (i.e., Gamma, and Gaussian with and without the log-transformation).

Zhang and Karunamuni [185] showed that the performance of the Beta kernel estimator is very similar to that of the reflection estimator of Schuster [155], which does not have the boundary problem only for densities exhibiting a shoulder condition at the endpoints of the support. For densities not exhibiting a shoulder condition, they showed that the performance of the Beta kernel estimator at the boundary was inferior to that of the well-known boundary kernel estimator, see, e.g., [55, 56, 183, 184] and references therein.

Bouezmarni and van Bellegem [14] introduced the idea of using Beta kernels to estimate the spectral density of long memory time series. Their technical report was recently updated and extended to include the case of short memory time series, and published as [23]. The asymptotics of the pointwise bias and variance for the spectral density estimator were obtained, as well as the uniform weak consistency on compacts and the relative weak consistency (i.e., the convergence to one, in probability, of the ratio of the estimator to the target density). A cross-validation method was also studied for
the selection of the bandwidth parameter \( b \) following the general method of Hurvich [83]. The authors show that the estimator has a better boundary behavior than traditional methods.

Bertin and Klutchnikoff [11] considered Beta kernel estimators for the estimation of density functions in \( \beta \)-Hölder spaces and under \( L^p \) losses. They showed that the estimator is minimax whenever \( 0 < \beta \leq 2 \) and \( 1 \leq p < 4 \), but not minimax otherwise. In particular, this means that Beta kernel estimators are minimax under \( L^2 \) losses if the target density is twice continuously differentiable (which is the most common assumption in the literature). These types of results are unique in the literature on asymmetric kernels; it would be interesting to see to what extent they hold for other asymmetric kernels. In [12], the same authors constructed a data-driven (also called adaptive) procedure of bandwidth selection, inspired by the method of Lepski [121], that achieves the minimax rate of convergence without a priori knowledge of the regularity \( \beta \) of the target density. They found that the procedure was competitive with the more common cross-validation methods, and the numerical computations were significantly faster.

In line with Igarashi and Kakizawa [90], Igarashi [84] considered an additive bias correction method of Schucany and Sommers [154] and the nonnegative bias correction methods of Terrell and Scott [172] and Jones and Foster [98], in the context of Beta kernel density estimators. Under the assumption that the target density is four-times continuously differentiable, the asymptotics of the pointwise bias, pointwise variance, MSE and MISE were found (the optimal rate of convergence was also shown to be \( O(n^{-8/9}) \) for the MISE and MSE inside \((0,1)\), instead of the usual \( O(n^{-4/5}) \)). In particular, the results partially complemented/extended/corrected those in [73]. The finite sample performance of the estimators was compared by computing the average and standard deviation of the integrated squared errors of Monte Carlo samples when the target density is a bimodal mixture of Beta densities.

Various other statistical topics related to Beta kernels are treated, for example, by Charpentier [26], Charpentier et al. [27], Charpentier and Oulidi [29], Funke and Hirukawa [53], Hirukawa et al. [75], Igarashi [87], Igarashi and Kakizawa [93], Jones and Henderson [100], Manivong [129], Yin and Hao [180].

When the density of the observations is not supported on the compact interval \([0,1]\), we can always apply a transformation to the data that maps to \([0,1]\) (for example, \( x \mapsto 1/(1+x) \) maps \([0,\infty)\) to \([0,1]\)) and then use Beta kernels. Another approach is to use asymmetric kernels that match the support of the target density directly. For instance, we have the following six common classes of asymmetric kernels on \([0,\infty)\): Gamma, Inverse Gamma, Inverse Gaussian, Birnbaum Saunders, Log-Normal and Reciprocal Inverse Gaussian. Many of the results that are proved for Beta kernels have been extended to these classes (or could be extended without much trouble), so we just list the relevant papers here instead of repeating every point above:

- Gamma kernels, see, e.g., [15, 18–22, 36, 37, 42, 43, 47, 49, 51, 53, 72, 77, 78, 91, 93, 95, 117, 127, 132–134, 160, 162, 164, 182];
- Inverse Gamma kernels, see, e.g., [107, 114, 137, 138, 140];
- Inverse Gaussian kernels, see, e.g., [22, 89, 93, 103, 116, 117, 122, 150, 152, 177];
- Birnbaum-Saunders kernels, see, e.g., [33, 89, 96, 104, 105, 130, 151, 187, 189, 193];
- Log-Normal kernels, see, e.g., [28, 85, 96, 108, 117];
- Reciprocal Inverse Gaussian kernels, see, e.g., [22, 89, 152];

Other asymmetric kernel classes have been considered such as the Weibull, but not much theoretical work has been done in those cases. Beta kernels and the six kernel classes above are the most common in the literature.

As can be seen from the lists just above, one of the current weaknesses in the theory of asymmetric kernels is the segmentation of the results by the specific form of the kernel. Fortunately, this concern has been addressed in recent years and a theory of so-called associated kernels has been developed (through many articles written by Célestin Kokonendji and his co-authors) to unify the theory of asymmetric kernels with the one for traditional kernels in both the univariate and multivariate settings, as well as treating discrete and continuous variants together. Associated kernels were developed and studied in the discrete setting first, see, e.g., [1, 7, 8, 71, 109–111, 113, 158, 161, 163, 175, 190, 192], then came the continuous univariate associated kernels, see Kokonendji and Libengué Dobélé-Kpoka [108], and finally multivariate associated kernels (discrete and continuous), see Kokonendji and Somé [111, 112]. The case of multivariate continuous associated kernels is the only one relevant to us in the present paper, so let us briefly mention the main contributions from Kokonendji and Somé [111, 112]. In those papers, the definition of associated kernels was extended to the multivariate setting (the explicit definition is given around Equation 3 below). In particular, the definition is broad enough that it covers all the asymmetric kernel classes mentioned in the paragraph above, as well as various multivariate generalizations treated in the literature and also traditional multivariate kernels (such as the ubiquitous Gaussian kernel, for example). In the two papers, the authors showed how associated kernels with a given correlation structure can be constructed using a variant of the mode-dispersion method, see [111, p.115-116], and they derived asymptotic expressions for the pointwise bias and variance of the corresponding smoothing estimator, see [111, Proposition 2.9] and [112, Proposition 2]. In [111],
they also showed how to modify the estimator near the boundary to reduce the pointwise bias even more, similarly to the modified Beta kernel estimator introduced by Chen [34]. In [112] (see [110] for the discrete case), a semiparametric approach adapted from Hjort and Glad [80] was applied when the associated kernel is parametrized by another (possibly multidimensional) parameter $\theta$, and asymptotics for the pointwise bias was also derived in this case. Specific examples are treated in both papers to illustrate the wide applicability of associated kernels to the currently segmented literature on asymmetric kernels and related estimators. In Section 3, the definition of multivariate associated kernels will be given and we will see that Dirichlet kernels are just a special case. However, most of the asymptotic results in Section 4 cannot be deduced from those in [111, 112], so significant work remains to be done.

Various other statistical topics related to asymmetric kernels are treated, for example, in [10, 13, 30–33, 38, 44, 45, 48, 50, 52, 54, 61, 62, 64, 65, 70, 74, 76, 79, 82, 86, 90, 92, 94, 106, 108, 115, 117, 123, 124, 128, 131, 135, 139, 143, 146, 167, 170, 176, 178, 179, 181, 186, 188, 191].

It should mentioned that Bernstein density estimators, studied theoretically, among other authors, by Vitale [174], Gawronski and Stadtmüller [58, 59, 60], Stadtmüller [165], Gawronski [57], Tenbusch [171], Babu et al. [4], Kakizawa [102], Babu and Chaubey [5], Bouezmarni and Rolin [17], Leblanc [118, 119], Igarashi and Kakizawa [88], Lu [126], Belalia [9], Ouimet [142, 144, 145], Hanebeck [68], Hanebeck and Klar [69] and Liu and Ghosh [125], share many of the same asymptotic properties (with proper reparametrization). As such, the literature on Bernstein estimators has paralleled that of Beta kernel estimators and other asymmetric kernel estimators in the past twenty years. For an overview of the vast literature on Bernstein estimators, we refer the interested reader to Ouimet [142].

3. Dirichlet kernels: definition and properties

The $d$-dimensional simplex and its interior are defined by

$$ S_d := \{ s \in [0,1]^d : \|s\|_1 \leq 1 \} \quad \text{and} \quad \text{Int}(S_d) := \{ s \in (0,1)^d : \|s\|_1 < 1 \}, $$

where $\|s\|_1 := \sum_{i=1}^d |s_i|$ and $d \in \mathbb{N}$. For $\alpha_1, \ldots, \alpha_d, \beta > 0$, the density of the Dirichlet$(\alpha, \beta)$ distribution is

$$ K_{\alpha,\beta}(s) := \frac{\Gamma(\|\alpha\|_1 + \beta)}{\Gamma(\beta) \prod_{i=1}^d \Gamma(\alpha_i)} \cdot (1 - \|s\|_1)^{-\beta-1} \prod_{i=1}^d s_i^{\alpha_i-1}, \quad s \in S_d. \quad (1) $$

For a given bandwidth parameter $b > 0$, and a sample of i.i.d. observations $X_1, \ldots, X_n$ that are $F$ distributed ($F$ is unknown) with a density $f$ supported on $S_d$, the Dirichlet kernel estimator is defined by

$$ \hat{f}_{a,b}(s) := \frac{1}{n} \sum_{i=1}^n K_{a+b+1,1-\|X_i\|_1+b+1}(X_i), \quad s \in S_d. \quad (2) $$

Two smoothing examples are given in Fig. 1 with $d = 2$, where the two subfigures on the left-hand side illustrate the target densities, and the two subfigures on the right-hand side show the corresponding estimates. The reader can also see that the shape of the kernel changes with the position $s$ on the simplex; this is in contrast with traditional estimators where the kernel is the same for every point. This variable smoothing allows Dirichlet kernel estimators (and more generally, asymmetric kernel estimators) to avoid the boundary bias problem of traditional kernel estimators.

Note that the estimator $\hat{f}_{a,b}$ is not a proper density since it does not integrate to 1 exactly, but it does integrate to 1 asymptotically. To prove this, denote Bulk := $\{ x \in S_d : |x_i - r_i| \leq (1/b + d + 1)^{1/2} b^{-1/2} / d \forall i \in \{1, \ldots, d\} \}$ where $r_i := (s_i+b)/(1+b(d+1))$, $x_{d+1} := (n-1||x||_1)/n$, $s_{d+1} := (1-||x||_1)/n$, and $X_1, \ldots, X_n \in$ Bulk with probability $1 - O(n \exp(-b^{-1/2})), as n \to \infty$, by a straightforward union bound and concentration argument (see [143, Equation (21)]), which is $1 - o(1)$ as long as $b = o((\log n)^{-3})$ (this is a very weak assumption given that $b_{opt} \propto n^{-2/(d+d)}$ in Theorem 2 below). Therefore, by the multivariate normal approximation for the Dirichlet$(\alpha = s + b, \beta = 1 - ||x||_1 + b)$ density derived in [143, Theorem 1], we have, as $n \to \infty$,

$$ \int_{S_d} f_{a,b}(s)ds = \frac{1}{n} \sum_{i=1}^n \int_{S_d} K_{a+b+1,1-||X_i||_1+b+1}(X_i) ds + o_P(1) $$

$$ = \frac{1}{n} \sum_{i=1}^n \int_{\text{Bulk}} \exp\left(-\frac{1}{2} \delta_X^\top \Sigma_r^{-1} \delta_X\right) \frac{1}{\sqrt{2\pi}^d |\Sigma_r|^{1/2}} \frac{1}{(1+b(d+1))^{1/2}} ds + o_P(1) \quad \text{with} \quad \delta_X := \frac{X_i - r}{\sqrt{1/b + d + 1}}, \quad \Sigma_r := \text{diag}(r) - rr^\top $$

$$ = \frac{1}{n} \sum_{i=1}^n \int_{\text{Bulk}} \exp\left(-\frac{1}{2} \delta_X^\top \Sigma_r^{-1} \delta_X\right) \frac{1}{\sqrt{2\pi}^d} ds + o_P(1) = 1 + o_P(1), $$

where the second to last equality follows from the change of variables $z = \delta_X \Sigma_r^{-1/2}$ and the fact that the symmetric positive definite matrix $\Sigma_r$ has determinant $\left(1 - \|r\|_1\right) \prod_{i=1}^d r_i$ by Tanabe and Sague [169, Theorem 1].
Fig. 1: Two-dimensional examples of contour plots for two target densities $f$ (left) and their respective estimate $\hat{f}_{n,b}$ (right), using Dirichlet kernels with $n = 10000$ and $b = n^{-1/3}$. The first target density (top left) is the mixture $0.4 \cdot \text{Dirichlet}(1.3, 1.6, 1) + 0.6 \cdot \text{Dirichlet}(1.7, 1.2, 2.5)$, whereas the second target density (bottom left) is the mixture $0.4 \cdot \text{Dirichlet}(4, 1, 2) + 0.6 \cdot \text{Dirichlet}(1, 3, 2)$.

Under mild regularity conditions, we will prove several asymptotic results for $\hat{f}_{n,b}$ in this paper: pointwise bias and variance, mean squared error (MSE), mean integrated squared error (MISE), mean integrated absolute error (MIAE), uniform strong consistency and asymptotic normality. The results are stated in Section 4 and proved in Section 6.

As mentioned in Section 2, Dirichlet kernels are continuous multivariate associated kernels. To see this, here is the definition, which can be found in [111, Definition 2.1] and [112, Definition 1]. In the continuous case, multivariate associated kernels are defined as density functions $K_{x,H}$ supported on a subset of $[0, \infty)^d$ (denoted by $T^d_+$), that are parametrized by points $x$ in the support and a bandwidth matrix $H$ which is symmetric and positive definite. As pointed out in [111, Table 2.1], the matrix $H$ can be full, diagonal or a Scott matrix (i.e., parametrized by a single parameter $h$), and must satisfy the following crucial property: For $Z_{x,H}$ a $d$-dimensional random vector which is $K_{x,H}$-distributed, then as $H \to 0_+$,

$$E[Z_{x,H}] - x = a(x, H) \to 0_-, \quad \text{Cov}(Z_{x,H}) = B(x, H) \to 0_+^d.$$  

(This definition extends naturally to the discrete setting, and it is also possible to have a mix of discrete and continuous components for $Z_{x,H}$.) Under this definition, and under relatively weak regularity conditions on the target density $f$ (see [112, p.167]), the asymptotics of the pointwise bias and variance for the corresponding estimator, denoted by $\hat{f}_{n,H}(x) = n^{-1} \sum_{i=1}^{n} K_{x,H}(X_i)$, were shown by Kokonendji and Somé [111, 112] to be, for any given $x \in T^d_+$,

$$\text{Bias}(\hat{f}_{n,H}(x)) = \nabla f(x)^\top a(x, H) + \frac{1}{2} \text{tr} \left[ \text{Hessian}(f)(x) \left\{ B(x, H) + a(x, H)^\top a(x, H) \right\} \right] + o(\text{tr}(B(x, H))),$$

$$\text{Var}(\hat{f}_{n,H}(x)) = n^{-1} f(x) \int_{T^d_+} K_{x,H}^2(u) du + o_{\text{r}} \left( \frac{n^{-1}}{(\text{det}(H))^{\gamma x}} \right),$$

with $r_x := \inf \{ t > 0 : \liminf_{n \to \infty} \int_{T^d_+} K_{x,H}^2(u) du (\text{det}(H))^{-t} > 0 \}$. 


In order to obtain explicit expressions for the pointwise bias and variance for the Dirichlet kernel estimator (using Equation (3)), we can estimate the expectation and covariances of the random vector

$$\xi_s = (\xi_1, \ldots, \xi_d) \sim \text{Dirichlet}(\frac{t}{b} + 1, \frac{(1-|\|\|)}{b} + 1), \quad s \in S_d.$$  

For all $i, j \in [1, \ldots, d]$, straightforward calculations yield (see, e.g., Ng et al. [141, p.39] for (*)):

$$E[\xi_i] \propto \frac{s_i + b}{b + d + 1} = \frac{s_i}{s_i + b(1 - (d + 1)s_i) + O(b^2)},$$

$$\text{Cov}(\xi_i, \xi_j) \propto \frac{(s_i + b)(1 + b(d + 1))}{(b + d + 1)^2} = \frac{b(s_i + b)(1 + b(d + 1))}{(b + d + 1)^2} = bs_i(\mathbf{1}_{(\|\|)} - s_j) + O(b^2).$$

This shows that $\hat{f}_{n,b}$ is a multivariate associated kernel supported on $T_d = S_d$ according to Definition 2.1 in [111] (alternatively, Definition 1 in [112]). (In fact, the expression (4) even shows that our estimator $\hat{f}_{n,b}$ could be derived asymptotically, a posteriori, from the mode-dispersion method described in [111, p.115-116].) Consequently, under the assumption that $f$ is twice continuously differentiable on $S_d$, we can get the asymptotics of the pointwise bias and variance from (3) with $a(x, H) = b(1 - (d + 1)s_i) + O(b^2)$ and $B(x, H) = b(d + 1)$ and $O(b^2)$. The explicit expression we obtain for the pointwise bias is written in Theorem 1 (it is just a special case of the broader results obtained by Kokonenjdi and Somé [111, 112]). However, to be clear, the expression for the pointwise variance in Theorem 1 is more precise than the one we obtain from the above argument (the technical bound on the main part of the variance in Lemma 1 in particular is necessary to obtain the asymptotics of the MISE rigorously). Also, our expression for the pointwise variance in Theorem 1 only assumes that $f$ is Lipschitz continuous instead of twice continuously differentiable, and we even prove the asymptotics near the boundary, which does not follow from the results in Kokonenjdi and Somé [111, 112].

4. Main results

For each result in this section, one of the following two assumptions will be used:

- The density $f$ is Lipschitz continuous on $S_d$.  
- The density $f$ is twice continuously differentiable on $S_d$.  

Also, here are some notations we will use throughout the rest of the paper. The notation $u = O(v)$ means that $\lim \sup |u|/v < C < \infty$ as $b \to 0$ or $n \to \infty$, depending on the context. The positive constant $C$ can depend on the target density $f$ and the dimension $d$, but no other variable unless explicitly written as a subscript. The most common occurrence is a local dependence of the asymptotics with a given point $s$ on the simplex, in which case we would write $u = O_s(v)$. In a similar fashion, the notation $u = o(v)$ means that $\lim |u|/v = 0$ as $b \to 0$ or $n \to \infty$. Subscripts indicate which parameters the convergence rate can depend on. The symbol $\rightarrow$ over an arrow `$\to$' will denote the convergence in law (or distribution). We will use the shorthand $[d] := \{1, \ldots, d\}$ in several places. The bandwidth parameter $b = b(n)$ is always implicitly a function of the number of observations, the only exception being in Lemma 1 and its proof. Finally, we denote the expectation of $\hat{f}_{n,b}(s)$ by

$$f_0(s) := E[\hat{f}_{n,b}(s)] = \int_{S_d} f(x)K_{[b+1,1-|\|\|]+1/(b+1)}(x)dx.$$  

Alternatively, notice that if $\xi_s \sim \text{Dirichlet}(s/b + 1, (1 - |\|\|)/b + 1)$, then we also have the representation

$$f_0(s) = E[f(\xi_s)].$$

The asymptotics of the pointwise bias and variance for Beta kernel estimators were first computed by Chen [34]. The theorem below extends this to the multidimensional setting.

Theorem 1 (Pointwise bias and variance). Assume that (6) holds. We have, as $n \to \infty$ and uniformly for $s \in S_d$,

$$\text{Bias}[\hat{f}_{n,b}(s)] = f_0(s) - f(s) = b g(s) + o(b),$$

where

$$g(s) = \frac{2}{b + d + 1}.$$  

Proof. The proof is given in Appendix A.
where
\[
g(s) := \sum_{i \in [d]} (1 - (d + 1)s_i) \frac{\partial}{\partial s_i} f(s) + \frac{1}{2} \sum_{i,j \in [d]} s_i (1_{i = j} - s_j) \frac{\partial^2}{\partial s_i \partial s_j} f(s).
\]

Assume that (5) holds instead. For every subset of indices \( \mathcal{I} \subseteq [d] \), denote
\[
\psi(s) := \psi_0(s) \quad \text{and} \quad \psi_{\mathcal{I}}(s) := \left( 4 \pi \right)^{d/2} \cdot (1 - ||s||_1) \prod_{i \in [d] \setminus \mathcal{I}} s_i \right)^{1/2}.
\]

Then, for any \( s \in \text{Int}(S_d) \), any subset \( \emptyset \neq \mathcal{I} \subseteq [d] \), and any \( \kappa \in (0, \infty)^d \), we have, as \( n \to \infty \),
\[
\text{Var}(\hat{f}_{n,b}(s)) = \begin{cases} 
 n^{-1} b^{-d/2} \cdot \left( (\psi(s)f(s) + O_b(b^{1/2})) \right), & \text{if } s_i/b \to \infty \forall i \in [d] \text{ and } (1 - ||s||_1)/b \to \infty, \\
 n^{-1} b^{-d(1 + 1/\mathcal{I})/2} \cdot \left( \psi_{\mathcal{I}}(s)f(s) \prod_{i \in \mathcal{I}} \frac{\Gamma(2\kappa_i + 1)}{\Gamma(2\kappa_i)} + O_{\kappa,s}(b^{1/2}) \right), & \text{if } s_i/b \to \kappa_i \forall i \in \mathcal{I}, s_i/b \to \infty \forall i \notin [d] \setminus \mathcal{I} \text{ and } (1 - ||s||_1)/b \to \infty.
\end{cases}
\]

This means that the pointwise variance is \( O_b(n^{-1} b^{-d/2}) \) in the interior of the simplex and it gets multiplied by a factor \( b^{-1/2} \) every time we go near the boundary in one of the \( d \) dimensions. If we are near an edge of dimension \( d - |\mathcal{I}| \), then the pointwise variance is \( O_b(n^{-1} b^{-d - 1/2}) \).

**Corollary 1** (Mean squared error). Assume that (6) holds. We have, as \( n \to \infty \) and for each \( s \in \text{Int}(S_d) \),
\[
\text{MSE}[\hat{f}_{n,b}(s)] := \mathbb{E}[|\hat{f}_{n,b}(s) - f(s)|^2] = \text{Var}(\hat{f}_{n,b}(s)) + \mathbb{E}[\hat{f}_{n,b}(s)]^2 = n^{-1} b^{-d/2} \cdot (\psi(s)f(s) + b^2 \cdot \varphi_1(s) + O_b(n^{-1} b^{-d + 1/2}) + o(b^2)).
\]

In particular, if \( f(s) \cdot g(s) \neq 0 \), the asymptotically optimal choice of \( b \), with respect to MSE, is
\[
b_{\text{opt}}(s) = n^{-2/(d+4)} \cdot \frac{d}{4} \cdot \frac{(\psi(s)f(s))^2}{\varphi_1(s)} \cdot b^{2/(d+4)},
\]
with
\[
\text{MSE}[\hat{f}_{n,b_{\text{opt}}}(s)] = n^{-4/(d+4)} \left[ 1 + \frac{d}{4} \cdot \frac{(\psi(s)f(s))^2}{\varphi_1(s)} \cdot b^{-d/(d+4)} + o(n^{-4/(d+4)}) \right].
\]

More generally, if \( n^{2/(d+4)} b \to \lambda \) for some \( \lambda > 0 \) as \( n \to \infty \), then
\[
\text{MSE}[\hat{f}_{n,b_{\text{opt}}}(s)] = n^{-4/(d+4)} \left[ \lambda^{-d/2} \cdot (\psi(s)f(s)) + \lambda^2 \cdot \varphi_1(s) + o(n^{-4/(d+4)}) \right].
\]

By integrating the MSE and showing that the contribution coming from points near the boundary is negligible, we obtain the following result.

**Theorem 2** (Mean integrated squared error). Assume that (6) holds. We have, as \( n \to \infty \),
\[
\text{MISE}[\hat{f}_{n,b}(s)] := \int_{S_d} \mathbb{E}[|\hat{f}_{n,b}(s) - f(s)|^2] ds = n^{-1} b^{-d/2} \int_{S_d} \psi(s)f(s) ds + b^2 \int_{S_d} \varphi_1(s) ds + o(n^{-1} b^{-d/2}) + o(b^2).
\]

In particular, if \( \int_{S_d} \varphi_1(s) ds > 0 \), the asymptotically optimal choice of \( b \), with respect to MISE, is
\[
b_{\text{opt}}(s) = n^{-2/(d+4)} \cdot \frac{d}{4} \cdot \frac{\int_{S_d} \psi(s)f(s) ds}{\int_{S_d} \varphi_1(s) ds} \cdot b^{2/(d+4)},
\]
with
\[
\text{MISE}[\hat{f}_{n,b_{\text{opt}}}(s)] = n^{-4/(d+4)} \left[ 1 + \frac{d}{4} \cdot \frac{\int_{S_d} \psi(s)f(s) ds}{\int_{S_d} \varphi_1(s) ds} \cdot b^{-d/(d+4)} + o(n^{-4/(d+4)}) \right].
\]

More generally, if \( n^{2/(d+4)} b \to \lambda \) for some \( \lambda > 0 \) as \( n \to \infty \), then
\[
\text{MISE}[\hat{f}_{n,b_{\text{opt}}}(s)] = n^{-4/(d+4)} \left[ \lambda^{-d/2} \cdot \int_{S_d} \psi(s)f(s) ds + \lambda^2 \cdot \int_{S_d} \varphi_1(s) ds + o(n^{-4/(d+4)}) \right].
\]
The following theorem is the analogue of the $L^1$ asymptotics first proved for traditional univariate kernel estimators by Hall and Wand [67], and then extended to the multivariate setting by Scott and Wand [157]. In the context of Beta kernels, the result can be found in Theorem 1 of [16]. As pointed out by Scott [156, Section 2.3.2], the MIAE enjoys many advantages over the MISE. It puts more emphasis on the tails of the target density, it is a dimensionless quantity, it is invariant to monotone changes of scale, and it is uniformly bounded (by 2). For a thorough study of the $L^1$ point of view in the kernel smoothing theory, we refer the reader to Devroye and Györfi [39].

**Theorem 3 (Mean integrated absolute error).** Assume that (6) holds. We have, as $n \to \infty$,

$$\text{MIAE}[\hat{f}_{n,b}] := \int_{S_d} \mathbb{E} \left| \hat{f}_{n,b}(s) - f(s) \right| ds = \int_{S_d} w(s) \mathbb{E} \left| Z - \frac{b g(s)}{w(s)} \right| ds + O(n^{-1} b^{-d/2}) + o(n^{-1/2} b^{-d/4}) + o(b),$$

where $w(s) := n^{-1/2} b^{-d/4} \sqrt{\psi(s)} f(s)$, $\psi$ and $g$ are defined in (9) and (8), and $Z \sim N(0,1)$. If $n^{1/2} b^{-d/4} \to \infty$, then we have the bound

$$\text{MIAE}[\hat{f}_{n,b}] \leq n^{-1/2} b^{-d/4} \sqrt{\frac{2}{\pi}} \int_{S_d} \sqrt{\psi(s)} f(s) ds + \frac{b}{\sqrt{\pi}} \int_{S_d} |g(s)| ds + o(n^{-1/2} b^{-d/4}) + o(b),$$

In particular, if $\int_{S_d} |g(s)| ds > 0$, the asymptotically optimal choice of $b$, with respect to the mean integrated absolute error bound (11), is

$$b_{opt} = n^{-2/(d+4)} \left[ \frac{d}{4} \sqrt{\frac{2}{\pi}} \int_{S_d} \sqrt{\psi(s)} f(s) ds \right]^{d/(d+4)},$$

with

$$\text{MIAE}[\hat{f}_{n,b_{opt}}] \leq n^{-2/(d+4)} \left[ 1 + \frac{d}{4} \left( \frac{1}{\sqrt{\pi}} \int_{S_d} \sqrt{\psi(s)} f(s) ds \right)^{d/(d+4)} \right] + o(n^{-2/(d+4)}).$$

More generally, if $n^{2/(d+4)} b \to \lambda$ for some $\lambda > 0$ as $n \to \infty$, then

$$\text{MIAE}[\hat{f}_{n,b}] \leq n^{-2/(d+4)} \left[ \lambda^{-d/4} \int_{S_d} \sqrt{\psi(s)} f(s) ds + \lambda \int_{S_d} |g(s)| ds \right] + o(n^{-2/(d+4)}).$$

The uniform strong consistency was proved for traditional multivariate kernel estimators by Devroye and Penrod [41] and for Beta kernel estimators by Bouezmarni and Roin [16]. In order to keep a control on the partial derivatives of the Dirichlet density $K_{\alpha,\beta}$ with respect to the parameters $\alpha_1, \ldots, \alpha_d, \beta$ in our proof, we add a small buffer to the boundary that goes to zero as $n \to \infty$. Our proof is completely different from the proof of the case $d = 1$ by Bouezmarni and Roin [16] (it is not clear how to generalize it) and instead relies on a novel chaining argument.

**Theorem 4 (Uniform strong consistency).** Assume that (5) holds. We have, as $n \to \infty$,

$$\sup_{s \in S_d} |\hat{f}_n(s) - f(s)| = O(b^{1/2}).$$

Furthermore, for $\delta > 0$, define

$$S_d(\delta) := \{ s \in S_d : 1 - \|s\| \geq \delta \text{ and } s_i \geq \delta \forall i \in [d] \}.$$

Then, if $b^{-d} \leq n$ as $n \to \infty$, we have

$$\sup_{s \in S_d(\delta)} |\hat{f}_n(s) - f(s)| = O \left( \frac{|\log n|^{3/2}}{b^{d+1/2} \sqrt{n}} \right) + O(b^{1/2}), \quad \text{a.s.}$$

In particular, if $|\log b^2| b^{-d-1} = o(n/(\log n)^3)$ as $n \to \infty$, then

$$\sup_{s \in S_d(\delta)} |\hat{f}_n(s) - f(s)| \to 0, \quad \text{a.s.}$$
A straightforward verification of the Lindeberg condition for double arrays yields the asymptotic normality. This result was never proved even for Beta kernel estimators.

**Theorem 5** (Asymptotic normality). Assume that (5) holds. Let $s \in \text{Int}(S_d)$ be such that $f(s) > 0$. If $n^{1/2}b^{d/4} \to \infty$ as $n \to \infty$ and $b \to 0$, then

$$n^{1/2}b^{d/4} \left( \hat{f}_{n,b}(s) - f(s) \right) \xrightarrow{D} N(0, \psi(s)f(s)).$$

If we also have $n^{1/2}b^{d/4+1/2} \to 0$ as $n \to \infty$ and $b \to 0$, then (12) of Theorem 4 implies

$$n^{1/2}b^{d/4} \left( \hat{f}_{n,b}(s) - f(s) \right) \xrightarrow{D} N(0, \psi(s)f(s)).$$

Independently of the above rates for $n$ and $b$, if we assume (6) instead and $n^{2/(d+4)}b \to \lambda$ for some $\lambda > 0$ as $n \to \infty$ and $b \to 0$, then the pointwise bias result in Theorem 1 implies

$$n^{2/(d+4)} \left( \hat{f}_{n,b}(s) - f(s) \right) \xrightarrow{D} N(\lambda g(s), \lambda^{-d/2}\psi(s)f(s)).$$

**Remark 1.** The rate of convergence for the $d$-dimensional kernel density estimator with i.i.d. data and bandwidth $h$ is $O(n^{-1/2}h^{-d/2})$ in Theorem 3.1.15 of Prakasa Rao [148], whereas $\hat{f}_{n,b}$ converges at a rate of $O(n^{-1/2}b^{-d/4})$. Hence, the relation between the bandwidth of $\hat{f}_{n,b}$ and the bandwidth of the traditional multivariate kernel density estimator is $b \approx h^2$.

5. Case study: minerals processing

Minerals processing is a branch of engineering that deals with the design and optimization of systems for beneficiation of valuable minerals out of ore rock materials. These ores are first comminuted to generate simple particles (formed by the least number of minerals possible, ideally, only one mineral), and then subjected to physical/physico-chemical separation processes. Here, an input stream of mixed particles (or feed) is separated into two or more product streams with, hopefully, purer composition. These processes can be studied at the particle level, in which case one or more (estimates) for each particle its probability of landing on each one of the possible output streams, as a function of one or more of its properties: for two output streams and one single property, these functions are called Tromp curves [173]. Schach et al. [153] generalized the tool in a nonparametric way to two properties $(X, Y)$, by estimating for each output stream $i$ the probability density function $f_{i,b,b}(x, y)$ using a bivariate kernel with bandwidth $(b_x, b_y)$, and then forcing at each point $(x, y)$ the set of estimated densities to sum to one. The procedure is essentially equivalent to linear discriminant analysis where the hypothesis of normality of the covariables is superseded by using kernel density estimates.

Kernel density estimates on the simplex allow the obvious generalization of this idea to obtain discrimination rules (in general) and multidimensional Tromp maps (in this specific case) for compositional covariables. To illustrate the idea, we use freely available particle data from an Apatite flotation experiment [81], for which we have available information about 2,825,712 particles, split into two output streams (the value stream and the waste stream). Flotation is a powerful physico-chemical concentration process that is particularly sensitive to the surface composition (i.e., the proportion of each mineral on the surface of a particle). Out of the 25 minerals considered, we formed 5 groups depending on their characteristics and process behaviour in contrast with the value mineral (see Pereira et al. [147] for details): “Apatite” (the value mineral), “semi-soluble salts” (with a similar chemical behavior than Apatite), “phyllosilicates” or sheet silicates (with a specific hydrodynamic behaviour), “other silicates” (waste, non-floaters), and “other minerals” (mostly sulfides, fast floating minerals often polluting the value stream).

Due to the preliminary comminution step, most of these particles are monomineralic ($> 86\%$) or bimineralic ($> 98\%$). Three or less minerals show $> 99.8\%$ of the particles. Shortly, most of these compositions are plagued with zeros, making it an ideal case for Dirichlet kernel methods (recall that the estimator does not spill over the simplex and it is asymptotically unbiased with an error that is uniform on the simplex by Theorem 1, including the boundary). We estimated the density (using Equation 2) for each $S_2$ side of the $S_3$ simplex that involve Apatite, the value mineral. For each ternary diagram, a regular grid of 100 $\times$ 100 nodes was constructed, those observations being zero for all three components were filtered out, and a small $\epsilon$ was added to all selected data, i.e., we computed (Equation 2) with $X_i' = aX_i + \epsilon I$ with $a$ such that $1^T X_i' = 1$, i.e., the data are re-closed to sum to 1. This was done to avoid the collapse of the Dirichlet kernels when an observation is exactly zero. $\epsilon$ was chosen to be half the grid step. This treatment is reasonable both given the observation mechanism of this data [81, 147] and the regularity and the bias-stability properties of the estimator proven in Theorem 1 and Theorem 4. The resulting density estimates are displayed in Fig. 3, both in raw and log scale, showing a strong concentration at the vertices and sides of the simplex: note the intense color of the pixel nearest to $(0, 0)$, corresponding to pure Apatite particles. Notice that the estimated density is strictly contained within the simplex, and it is not spilling over beyond its boundaries: this is particularly important given the strong concentration of data at the sides of the simplex.
Fig. 2: Tromp curves on the simplex for the system Apatite-semisolubles-phyllosilicates-other silicates-other minerals (red: high probability of going to value stream; blue: high probability of going to waste stream).

Fig. 2 shows the results of the calculations for the Tromp simplicial maps, i.e.,

\[ T_b(s) = \frac{f^{(v)}_{n,b}(s)}{f^{(v)}_{n,b}(s) + f^{(w)}_{n,b}(s)}, \]

where the superindexes \(^{(v)}\) and \(^{(w)}\) represent the density for the value stream and for the waste stream, respectively. It can be seen that particles formed by less than \(\sim 70\%\) Apatite quickly develop high probabilities of landing in the waste stream. Particles with high proportion of Apatite (\(> 80\%\)) land in the value stream. The complexity of the dependence of the Tromp map on the proportion of phyllosilicates (seen in all diagrams involving this component) suggests the interplay of several factors on top of just the Apatite purity, like, e.g., for particles mostly formed by these sheet silicates, where their hydrodynamics are dominated by their platy shape, and they stay longer in suspension and are transferred to the value stream. Finally, the diagrams involving sulphide minerals ("other") show that the probabilities of these minerals to report to a specific output stream are much nearer to 0.5-0.5, indicating that the process is not less selective with respect to these minerals.
Fig. 3: Dirichlet kernel density estimates of particles on the value stream (concentrate, top, yellow to red) and on the waste stream (tailings, bottom, yellow to blue): the more intense the red/blue, the higher the density. Upper triangle plots show the log-density, lower triangle plots show the raw density. Each diagram shows data on the simplex (Apatite - variable on the column - variable on the row).
6. Proofs

6.1. Proof of Theorem 1

The expression for the pointwise bias follows from the last paragraph in Section 3. To obtain the asymptotics of the pointwise variance in the interior of the simplex, \( \text{Var}(\hat{f}_{n,b}(s)) = n^{-1}b^{-d/2} \cdot (\psi(s) f(s) + O_b(b^{1/2})) \), we could again refer to Kokonendji and Somé [111, 112] if we assumed (6), but here we need a slightly more precise result to get the asymptotics of the MISE later and we work under the weaker assumption (5) that \( f \) is Lipschitz continuous on \( S_d \). We also want the asymptotics near the boundary, which does not follow from the results of Kokonendji and Somé [111, 112]. For these reasons, we provide a proof below. First, note that we can write

\[
\hat{f}_{n,b}(s) - f_b(s) = \frac{1}{n} \sum_{i=1}^{n} Y_{i,b}(s),
\]

where the random variables

\[
Y_{i,b}(s) := K_{\frac{1}{d+1},\frac{1}{d+1}}(X_i) - f_b(s), \quad 1 \leq i \leq n, \quad \text{are i.i.d.}
\]

Hence, if \( \gamma_s \sim \text{Dirichlet}(2s/b + 1, 2(1 - \|s\|_1)/b + 1) \), then

\[
\text{Var}(\hat{f}_{n,b}(s)) = n^{-1} \mathbb{E} \left[ K_{\frac{1}{d+1},\frac{1}{d+1}}(X) \right] - n^{-1}(f_b(s))^2 = n^{-1} A_b(s) \mathbb{E}[f(\gamma_s)] - O(n^{-1})
\]

where

\[
A_b(s) := \Gamma(2(1 - \|s\|_1)/b + 1) \prod_{i \in [d]} \Gamma(2s_i/b + 1) \cdot \frac{\Gamma^2(1/b + d + 1)}{2^{(2d + 1)/2} \prod_{i \in [d]} \Gamma(2s_i/b + 1)}.
\]

and where the last line in (15) follows from the Lipschitz continuity of \( f \), the Cauchy-Schwarz inequality and the analogue of (4) for \( \gamma_s \):

\[
\mathbb{E}[f(\gamma_s)] - f(s) = \sum_{i \in [d]} O(\mathbb{E}[\|\gamma_i - s_i\|]) \lesssim \sum_{i \in [d]} O(\sqrt{\mathbb{E}[\|\gamma_i - s_i\|^2]}) = O(b^{1/2}).
\]

The conclusion of Theorem 1 follows from (15) and Lemma 1 below.

**Lemma 1.** We have, as \( b \to 0 \) and uniformly for \( s \in S_d \),

\[
0 < A_b(s) \leq \frac{b^{d+1/2} (1/b + d^{d+1/2})}{4 \pi^{d/2} \sqrt{(1 - \|s\|_1/b) \prod_{i \in [d]} s_i}} (1 + O(b)).
\]

Furthermore, for any subset \( \emptyset \neq \mathcal{J} \subseteq [d] \), and any \( \kappa \in (0, \infty)^d \),

\[
A_b(s) = \begin{cases} 
\begin{aligned}
& b^{-d/2} \psi(s)(1 + O_b(b)), & \text{if } s_i/b \to 0 \quad \forall i \in [d] \text{ and } (1 - \|s\|_1/b) \to \infty, \\
& b^{-d+|\mathcal{J}|/2} \psi_{\mathcal{J}}(s) \prod_{i \in \mathcal{J}} R_{2s_i/b}^{(2(s_i/b) - \psi_{\mathcal{J}}(s)) \sum_{i \in \mathcal{J}} [2(s_i/b) - \psi_{\mathcal{J}}(s)]} (1 + O_{\kappa,b}(b)), & \text{if } s_i/b \to \kappa \quad \forall i \in \mathcal{J} \text{ and } s_i/b \to \infty \quad \forall i \in [d] \setminus \mathcal{J} \\
& b^{-d+|\mathcal{J}|/2} \psi_{\mathcal{J}}(s) \prod_{i \in \mathcal{J}} R_{2s_i/b}^{(2s_i/b) - \psi_{\mathcal{J}}(s)) \sum_{i \in \mathcal{J}} [2s_i/b - \psi_{\mathcal{J}}(s)]} (1 + O_{\kappa,b}(b)), & \text{if } s_i/b \to \kappa \quad \forall i \in \mathcal{J} \text{ and } s_i/b \to \infty \quad \forall i \in [d] \setminus \mathcal{J}
\end{aligned}
\end{cases}
\]

where \( \psi \) and \( \psi_{\mathcal{J}} \) are defined as in (9).

**Proof of Lemma 1.** If we denote

\[
S_b(s) := \frac{R^2((1 - \|s\|_1/b) \prod_{i \in [d]} R^2(s_i/b))}{R^2(2 - \|s\|_1/b) \prod_{i \in [d]} R^2(2s_i/b)} \cdot \frac{R(2/b + d)}{R^2(1/b + d)},
\]

where

\[
R(z) := \frac{\sqrt{2\pi} e^{-z^2/2} z^{d + 1/2}}{\Gamma(z + 1)}, \quad z \geq 0,
\]

then, for all \( s \in \text{Int}(S_d) \), we have

\[
A_b(s) = \frac{2^{2(1-\|s\|_1/b+1/2)} \prod_{i \in [d]} 2^{2s_i/b+1/2}}{(2\pi)^{d+1/2} \sqrt{(1 - \|s\|_1/b) \prod_{i \in [d]} s_i/b}} \cdot \frac{\sqrt{2\pi} e^{-d(1/b + d)^2/2b + 1}}{(2/b + d)^{2d+1/2}} \cdot S_b(s).
\]
where
\[
A_b(s) = \frac{\Gamma(2\kappa_i + 1)}{\Gamma^2(\kappa_i + 1)} \left(1 + O_{\kappa_i}(b)\right) = \frac{\Gamma(2\kappa_i + 1)}{\Gamma^2(\kappa_i + 1)} \left(1 + O_{\kappa_i}(b)\right).
\] (21)

Next, let \( \Theta \neq \mathcal{J} \subseteq [d] \) and \( \kappa \in (0, \infty)^d \). If \( s_i/b \to \kappa_i \) for all \( i \in \mathcal{J} \), \( s_i/b \to \infty \) for all \( i \in [d] \setminus \mathcal{J} \) and \( (1 - \|s_i\|)/b \to \infty \), then, from (16),

\[
A_b(s) = \prod_{i \in \mathcal{J}} \frac{\Gamma(2\kappa_i + 1)}{\Gamma^2(\kappa_i + 1)} \left(1 + O_{\kappa_i}(b)\right) = \frac{\Gamma(2\kappa_i + 1)}{\Gamma^2(\kappa_i + 1)} \left(1 + O_{\kappa_i}(b)\right).
\] (21)

Similarly to (21), Stirling’s formula and (20) imply

\[
A_b(s) = \prod_{i \in \mathcal{J}} \frac{\Gamma(2\kappa_i + 1)}{2^{\kappa_i + 1/2} \Gamma(\kappa_i + 1)} \left(1 + O_{\kappa_i}(b)\right) = \frac{\Gamma(2\kappa_i + 1)}{2^{\kappa_i + 1/2} \Gamma(\kappa_i + 1)} \left(1 + O_{\kappa_i}(b)\right).
\] (21)

This concludes the proof of Lemma 1 and Theorem 1. \( \Box \)

### 6.2. Proof of Theorem 2

By the bound (17), the fact that \( f \) is uniformly bounded (it is continuous on \( S_d \)), the almost-everywhere convergence in (21), and the dominated convergence theorem, we have

\[
b^{-d/2} \int_{S_d} A_b(s) f(s) ds = \int_{S_d} \psi(s) f(s) ds + o(1).
\]

The expression for the pointwise variance in (15) (using Lemma 1), and the pointwise bias in (7), yield

\[
\text{MISE} \left[ \hat{f}_{b,h} \right] = \int_{S_d} \text{Var} \left[ \hat{f}_{b,h}(s) \right] + \text{Bias} \left[ \hat{f}_{b,h}(s) \right]^2 ds = n^{-1} b^{-d/2} \int_{S_d} \psi(s) f(s) ds + b^2 \int_{S_d} g^2(s) ds + o(n^{-1} b^{-d/2}) + o(b^2).
\]

This ends the proof.
6.3. Proof of Theorem 3

By Lemma 2 in [40], if \( \xi_1, \ldots, \xi_n \) is an i.i.d. sequence of random variables with \( \mathbb{E}[|\xi_1|^3] < \infty \), then

\[
\sup_{a \in \mathbb{R}} \left| \mathbb{E}[\xi_a] - \mathbb{E}[\xi_a] - a \right| \leq \sqrt{\text{Var}(\xi_a)} \mathbb{E}[|Z - a|] \leq c_0 \frac{\mathbb{E}[|\xi_1| + \mathbb{E}[|\xi_1|^3]}{n \text{Var}(\xi_1)},
\]

(22)

where \( \tilde{\xi}_n := \frac{1}{n} \sum_{i=1}^n \xi_i \), \( Z \sim N(0,1) \), and \( c_0 = c_0(d) > 0 \) is a constant that depends only on \( d \). By applying this result with \( \xi_i := K_{s+i\lambda}X_i \) (here, \( s \in \text{Int}(S_d) \) is fixed) and \( a^*(s) := (f(s) - \mathbb{E}[\hat{f}_{n,b}(s)])/(\text{Var}(\hat{f}_{n,b}(s)))^{1/2} \), we can show

\[
\mathbb{E}[|\hat{f}_{n,b}(s) - f(s)|] - \sqrt{\text{Var}(\hat{f}_{n,b}(s))} \mathbb{E}[|Z - a^*(s)|] \leq c_1 n^{-1/2}d^{-d/4} \psi(s),
\]

(23)

for another constant \( c_1 = c_1(d) > 0 \) that depends only on \( d \). Indeed, to get the last inequality, note that, as \( n \to \infty \),

\[
\frac{\mathbb{E}[|\xi_1| - \mathbb{E}[|\xi_1|^3]}{\mathbb{E}[|\xi_1|^3]} \leq \frac{4 [\mathbb{E}[|\xi_1|^2] + (\mathbb{E}[|\xi_1|^3])^2]}{[\mathbb{E}[|\xi_1|^2] - (\mathbb{E}[|\xi_1|^3])^2} = 4 \frac{\mathbb{E}[|\xi_1|^2]}{\mathbb{E}[|\xi_1|^3]} + O(1),
\]

by applying Jensen’s inequality. Similarly to the proof of Theorem 1 (which includes Lemma 1), we have

\[
\frac{\mathbb{E}[|\xi_1|^2]}{\mathbb{E}[|\xi_1|^3]} = \tilde{A}_b(s) (1 + O(b^{1/2})),
\]

(24)

where

\[
\tilde{A}_b(s) := \frac{\Gamma(3(1 - ||s||_1)/b + 1)}{\Gamma(2(1 - ||s||_1)/b + 1) \Gamma(1 - ||s||_1)/b + 1)} \prod_{i \in [d]} \frac{\Gamma(3s_i/b + 1)}{\Gamma(2s_i/b + 1) \Gamma(s_i/b + 1)} \frac{\Gamma(2b + 1) \Gamma(1/b + 1)}{\Gamma(3/b + b + 1)}. \]

Following the first part of the proof of Lemma 1, it is straightforward to show that

\[
\tilde{A}_b(s) \leq \frac{3^{b(1 - ||s||_1)/b + 1/2}}{2^{b(1 - ||s||_1)/b + 1/2} \sqrt{(1 - ||s||_1)/b}} \prod_{i \in [d]} \frac{3^{s_i/b + 1/2}}{3^{s_i/b + 1/2} \sqrt{s_i/b}} \sqrt{2} \pi \epsilon d(2b + 1) \prod_{i \in [d]} \frac{3^{b/d + 1/2}}{b^{d/2 + 1/2} (3/b + d)^{b/d + 1/2}} (1 + O(b))
\]

\[
= \frac{b^{d+1/2} \sqrt{(1 - ||s||_1)/b} \prod_{i \in [d]} s_i}{b^{d/2} (1 + O(b))(3/b + d)^{1/2}} \left( \frac{3/b + d/2}{3/b + d} \right)^{b/d + 1/2} e^{-d} \left( \frac{3/b + d/2}{3/b + d} \right)^{b/d + 1/2} e^{-d}
\]

(25)

Hence, putting (22), (24) and (25) together proves (23).

Now, by (23), the triangle inequality and the fact that \( \psi \) is integrable on \( S_d \) yield

\[
\left| \text{MIAE}[\hat{f}_{n,b}] - \int_{S_d} w(s) \mathbb{E}[Z - \frac{b}{w(s)}] ds \right| \leq c_2 n^{-1/2}d^{-d/4} + \int_{S_d} \left| \sqrt{\text{Var}(\hat{f}_{n,b}(s))} \mathbb{E}[Z - a^*(s)] - w(s) \mathbb{E}[Z - \frac{b}{w(s)}] \right| ds,
\]

(26)

where \( w(s) := n^{-1/2}d^{-d/4} \sqrt{\psi(s)/f(s)} \) and \( c_2 = c_2(d) > 0 \) is a constant that depends only on \( d \). It was shown in Lemma 7 of Devroye and Penrod [40] that, for all \( u, w \geq 0 \) and all \( v, z \in \mathbb{R} \),

\[
|u| \mathbb{E}[Z - \frac{v}{w}] - w \mathbb{E}[Z - \frac{u}{w}] \leq \sqrt{2} \pi |u - w| + |v - z|,
\]

so the right-hand side of (26) is bounded from above by

\[
c_2 n^{-1/2}d^{-d/4} + \int_{S_d} \sqrt{\text{Var}(\hat{f}_{n,b}(s))} - \frac{\sqrt{\psi(s)/f(s)}}{n^{1/2}d^{-d/4}} ds + \int_{S_d} |\text{Bias}[\hat{f}_{n,b}(s)] - b \psi| ds.
\]

By the expression (15) for the pointwise variance (using Lemma 1), and the pointwise bias in (7), the above is \( O(n^{-1/2}d^{-2}) + O(n^{-1/2}d^{-2}) + o(b) \), which proves (10). The bound (11) is a direct consequence of (10) and the trivial bound \( \mathbb{E}|Z - u| \leq \sqrt{2/\pi} + |u| \). This ends the proof.
6.4. Proof of Theorem 4

This is the most technical proof, so here is the idea. The first three lemmas below bound, uniformly, the Dirichlet density (Lemma 2), the partial derivatives of the Dirichlet density with respect to the parameters $\alpha_1, \ldots, \alpha_d$ and $\beta$ (Lemma 3), and then the absolute difference of densities (pointwise and under expectations) that have different parameters (Lemma 4). This is then used to show continuity estimates for the random field $s \mapsto Y_{j, \beta}(s)$ from (14) (Proposition 1), meaning that we get a control on the probability that $Y_{j, \beta}(s)$ and $Y_{j, \beta}(s')$ are too far apart when $s$ and $s'$ are close. The proof of Proposition 1 relies on a novel chaining argument. From this, we easily deduce large deviation bounds for the supremum of $Y_{j, \beta}(s)$ over points $s'$ that are inside a small hypercube of width $2b$ centered at $s$ (Corollary 2). Since $f_{\alpha, \beta}(s) - f_{\beta}(s) = \frac{1}{2} \sum_{i=1}^n Y_{i, \beta}(s)$, we can estimate tail probabilities for the supremum of $f_{\alpha, \beta}(s) - f_{\beta}(s)$ over $S_d(bd)$ by union bound over the supremum on a collection of small hypercubes that partitions $S_d(bd)$ and apply a large deviation bound from Corollary 2 to each one of them.

In the first lemma, we bound the density of the Dirichlet($\alpha, \beta$) distribution from (1).

Lemma 2. If $\alpha_1, \ldots, \alpha_d, \beta \geq 2$, then

$$
\sup_{s \in S_d} K_{\alpha, \beta}(s) \leq \frac{||\alpha||! + \beta - 1}{(\beta - 1) \prod_{i=1}^d (\alpha_i - 1)} (||\alpha||! + \beta - d - 1)^d.
$$

Proof of Lemma 2. Whenever $\alpha_1, \ldots, \alpha_d, \beta \geq 2$, the Dirichlet density $K_{\alpha, \beta}$ is well-known to maximize at $s^* = (\alpha - 1)/(||\alpha||! + \beta - d - 1)$. At this point, we have

$$
K_{\alpha, \beta}(s^*) = \frac{\Gamma(||\alpha||! + \beta)}{\Gamma(\beta) \prod_{i=1}^d \Gamma(\alpha_i)} (\beta - 1)^{\beta - 1} \prod_{i=1}^d (\alpha_i - 1)^{\alpha_i - 1 - ||\alpha||!} (||\alpha||! + \beta - d - 1)^{||\alpha||! + \beta - d - 1}.
$$

(27)

From Theorem 2.2 in [6], we also know that, for all $y \geq 2$,

$$
\sqrt{2\pi e} (y - 1)^{y-1/2} \leq \Gamma(y) \leq \frac{2}{\sqrt{2\pi}} (y - 1)^{y-1/2}.
$$

Therefore, (27) is

$$
\leq \frac{2}{\sqrt{2\pi}} (2\pi)^{-d/2} \cdot e^{-d} \cdot \left(1 - \frac{d}{||\alpha||! + \beta - 1}\right) \cdot \left(\beta - 1\right)^{\beta - 1} \prod_{i=1}^d (\alpha_i - 1)^{\alpha_i - 1 - ||\alpha||!} (||\alpha||! + \beta - d - 1)^{||\alpha||! + \beta - d - 1}.
$$

$$
\leq \frac{2}{\sqrt{2\pi}} (2\pi)^{-d/2} \cdot e^{-d} \cdot \left(\beta - 1\right)^{\beta - 1} \prod_{i=1}^d (\alpha_i - 1)^{\alpha_i - 1 - ||\alpha||!} (||\alpha||! + \beta - d - 1)^{||\alpha||! + \beta - d - 1}.
$$

where we used our assumption $\alpha_1, \ldots, \alpha_d, \beta \geq 2$ and the fact that $(1 - y)^{-1} \leq e^{y^1}$ for $y \in [0, 1/2]$ to obtain the second inequality.

In the second lemma, we bound the partial derivatives of the Dirichlet($\alpha, \beta$) density with respect to its parameters.

Lemma 3. If $\alpha_1, \ldots, \alpha_d, \beta \geq 2$, then for all $s \in \text{Int}(S_d)$,

$$
\left| \frac{\partial}{\partial \alpha_j} K_{\alpha, \beta}(s) \right| \leq \left| \log(||\alpha||! + \beta) + \log(\alpha_j) + \log s_j \right| \cdot \sqrt{\frac{||\alpha||! + \beta - 1}{(\beta - 1) \prod_{i=1}^d (\alpha_i - 1)}} (||\alpha||! + \beta - d - 1)^d,
$$

(28)

$$
\left| \frac{\partial}{\partial \beta} K_{\alpha, \beta}(s) \right| \leq \left| \log(||\alpha||! + \beta) + \log(\beta) + \log(1 - ||\alpha||! - 1) \right| \cdot \sqrt{\frac{||\alpha||! + \beta - 1}{(\beta - 1) \prod_{i=1}^d (\alpha_i - 1)}} (||\alpha||! + \beta - d - 1)^d.
$$

(29)

Proof of Lemma 3. The digamma function $\psi(z) := \Gamma'(z)/\Gamma(z)$ satisfies $|\psi(z)| < |\log(z)|$ for all $z \geq 2$ (see, e.g., Lemma 2 in [136]). Hence, for all $j \in [d]$ and all $s \in \text{Int}(S_d)$,

$$
\left| \frac{\partial}{\partial \alpha_j} K_{\alpha, \beta}(s) \right| = \left(\psi(||\alpha||! + \beta) + \psi(\alpha_j) + \log s_j\right) K_{\alpha, \beta}(s) \leq \left| \log(||\alpha||! + \beta) + \log(\alpha_j) + \log s_j \right| K_{\alpha, \beta}(s).
$$

The conclusion (28) follows from Lemma 2. The proof of (29) is virtually identical, and thus omitted.

\[\square\]
As a consequence of Lemma 3 and the multivariate mean value theorem, we can control the absolute difference of two Dirichlet kernels with different parameters, pointwise and under expectations.

**Lemma 4.** If \( \alpha, \ldots, \alpha_d, \beta, \alpha', \ldots, \alpha'_d, \beta' \geq 2 \), and \( X \) is \( F \)-distributed with a bounded density \( f \) supported on \( S_d \), then

\[
\mathbb{E}[|K_{\alpha', \beta'}(X) - K_{\alpha, \beta}(X)|] \leq 3(d + 1)\|f\|_\infty \left\langle \left\langle \frac{|\alpha'\cap \beta'|}{|\alpha\cap \beta|} \right\rangle \right\rangle \cdot \left\langle \left\langle |\alpha\cap \beta|_{1 \rightarrow 1} + (\beta \wedge \beta') - d - 1 \right\rangle_{1 \rightarrow 1} \right\rangle \cdot \log \left( \left\langle \left\langle \alpha \cap \alpha' \right\rangle_{1 \rightarrow 1} + (\beta \wedge \beta') \right\rangle \right) \|f\|_\infty.
\]

where \( \alpha \cap \alpha' := (\max(\alpha, \alpha'))_{\in\{1, \ldots, d\}} \), \( \beta \wedge \beta' := \min(\beta, \beta') \). Furthermore, let

\[
S_d(\delta) := \{ s \in S_d : 1 - \|s\|_1 \geq \delta \text{ and } s_i \geq \delta \forall i \in [d] \}, \quad \delta > 0.
\]

Then, for \( 0 < \delta \leq e^{-1} \), we have

\[
\max_{s \in S_d(\delta)} |K_{\alpha', \beta'}(s) - K_{\alpha, \beta}(s)| \leq 3(d + 1)\|f\|_\infty \log \delta \cdot \left\langle \left\langle \frac{|\alpha'\cap \beta'|}{|\alpha\cap \beta|} \right\rangle \right\rangle \cdot \left\langle \left\langle |\alpha\cap \beta|_{1 \rightarrow 1} + (\beta \wedge \beta') - d - 1 \right\rangle_{1 \rightarrow 1} \right\rangle \cdot \log \left( \left\langle \left\langle \alpha \cap \alpha' \right\rangle_{1 \rightarrow 1} + (\beta \wedge \beta') \right\rangle \right) \|f\|_\infty.
\]

**Proof of Lemma 4.** By the triangle inequality and the multivariate mean value theorem,

\[
\mathbb{E}[|K_{\alpha', \beta'}(X) - K_{\alpha, \beta}(X)|] \leq \|f\|_\infty \int_{\text{Int}(S_d)} \left\langle \left\langle \frac{\partial}{\partial \beta} K_{\alpha, \beta}(s) \right\rangle_{\beta = \alpha, \beta} \right\rangle \left\langle |\beta - \beta'| + \sum_{j=1}^d \frac{\partial}{\partial \beta_j} K_{\alpha, \beta}(s) \right\rangle_{\beta = \alpha, \beta} \left\langle |\alpha_j - \alpha'_j| \right\rangle_{1 \rightarrow 1} ds,
\]

where, for every \( s \in \text{Int}(S_d) \), \((\alpha_s, \beta_s)\) is some point on the line segment joining \((\alpha, \beta)\) and \((\alpha', \beta')\). Now, by the estimates in Lemma 3, the above is

\[
\leq \|f\|_\infty \int_{S_d} |\log(1 - \|s\|_1)| ds + \sum_{j=1}^d \int_{S_d} |\log s_j| ds_j = 1.
\]

Together with (32), this proves (30). The proof of the second claim (31) follows from a simpler argument (without the integrals), and is left to the reader.

**Proposition 1** (Continuity estimates). Recall from (1) that

\[
Y_{i, \delta}(s) := K_{s, 1 + \frac{1}{n}}(X) - \mathbb{E} \left[ K_{s, 1 + \frac{1}{n}}(X) \right], \quad 1 \leq i \leq n.
\]

Let \( s \in S_d(b(d + 1)) \), \( n \geq 1 \), \( 0 < b < (e^{-16} \sqrt{d} \cdot d') \), \( 0 < \alpha \leq e^{-1}\|f\|_\infty \log b \cdot b^{d+1/2} \), and take the unique

\[
\delta \in (0, e^{-1} \log \log \log \log b) \text{ that satisfies } \delta \log \delta = \frac{b^{d+1/2} \alpha}{\|f\|_\infty \log b}.
\]

Then, for all \( h \in \mathbb{R} \),

\[
P \left( \sup_{s \in \mathbb{R}^{d+1}} \left| \frac{1}{n} \sum_{i=1}^n Y_{i, \delta}(s) \right| \geq h + \alpha \right) \leq \frac{1}{100^2 d^2\|f\|_\infty \log b} \left( \left( \log \log \log \log b \right) \right)^2.
\]

where \( C_{f,d} > 0 \) is a constant that depends only on the density \( f \) and the dimension \( d \).

**Proof of Proposition 1.** By a union bound, the probability in (35) is

\[
\leq P \left( \sup_{s \in \mathbb{R}^{d+1}} \left| \frac{1}{n} \sum_{i=1}^n Y_{i, \delta}(s) \right| \geq h + \alpha \right) \cap \left( \sum_{i=1}^n \left| I_{X \in S_d} \right| \leq n \cdot 4 \|f\|_\infty \delta \right) + P \left( \sum_{i=1}^n \left| I_{X \in S_d} \right| \geq n \cdot 4 \|f\|_\infty \delta \right) + P \left( \sup_{s \in \mathbb{R}^{d+1}} \left| \frac{1}{n} \sum_{i=1}^n Y_{i, \delta}(s) \right| \geq h + \alpha \right) =: (A) + (B) + (C).
\]
In order to bound the term \((A)\) in (36), note that our assumption \(s \in S_d(b(d + 1))\) and \(s' = s + [-b, b]^d\) imply \(s, s' \in S_d(b)\), which in turn implies
\[
\alpha_1 = \frac{(s_1)_1}{b} + 1, \ldots, \alpha_d = \frac{(s_d)_1}{b} + 1, \beta = \frac{1 - \|s\|_1}{b} + 1 \geq 2,
\]
and thus
\[
\sqrt{\|\alpha\|_1 + \beta - 1} \leq \sqrt{\|\alpha\|_1 + \beta - 1} = \sqrt{b^{-1} + d}.
\]
Together with our assumption in (34) and the upper bound on the Dirichlet density in Lemma 2, we have, on the event \(\|\sum_{i=1}^n 1_{x_i \in S_d(\delta)} \|_{\infty} \leq n \cdot 4 \|f\|_{\infty} \delta\),
\[
\left| \frac{1}{n} \sum_{i=1}^n (Y_{i, b}(s') - Y_{i, b}(s)) 1_{\{X_i \in S_d(\delta)\}} \right| \leq 4 \cdot 4 \|f\|_{\infty} \delta \cdot b^{-d} \sqrt{b^{-1} + d} \leq \frac{16 \sqrt{1 + bd}}{|\log \delta| |\log b|} a.
\]
Since \(0 < \delta \leq e^{-1}\) and \(0 < b < (e^{-16} n^2 \wedge d^{-1})\) by assumption, the above is \(< a\), which means that
\[
(A) = 0.
\]

The term \((B)\) is the probability that there are “too many bad observations” (i.e., too many \(X_i\)’s near the boundary of the simplex, where the partial derivatives of the Dirichlet density with respect to \(\alpha_1, \ldots, \alpha_d\) and \(\beta\) explode). We will control this term with a concentration bound. First, note that the volume of \(S_d(b)\) is almost-surely continuous, and by assumption, the above is valid for all \(\alpha_1, \ldots, \alpha_d \geq -1\). From (38) and the fact that \(\|f\|_{\infty}\) is finite (\(f\) is continuous by assumption and \(S_d(b)\) is compact), we get that
\[
E[1_{\{X_i \in S_d(\delta)\}}] \leq \frac{2(\|f\|_{\infty} \delta)}{(d - 1)!}.
\]
By applying Hoeffding’s inequality and condition (34), we obtain
\[
(B) \leq \exp \left(-2n \cdot \left(2(d - 1)! - 1\right) \cdot \frac{2\|f\|_{\infty}}{(d - 1)!} \delta^2 \right) \leq \exp \left(-2 \left(\frac{n^{1/2} b^{d+1/2}}{|\log \delta| |\log b|} a \right)^2\right).
\]
Now, in order to bound the third probability in (36), the main idea of the proof is to decompose the supremum with a chaining argument and apply concentration bounds on the increments at each level of the \(d\)-dimensional tree. With the notation \(\mathcal{H}_k := 2^{-k} \cdot b \mathbb{Z}^d\), we have the embedded sequence of lattice points
\[
\mathcal{H}_0 \subset \mathcal{H}_1 \subset \cdots \subset \mathcal{H}_k \subset \cdots \subset \mathbb{R}^d.
\]
Hence, for \(s \in S_d(b(d + 1))\) fixed, and for any \(s' \in [-b, b]^d\), let \((s_k)_{k \in \mathbb{N}}\) be a sequence that satisfies
\[
s_0 = s, \quad s_k - s \in \mathcal{H}_k \cap [-b, b]^d, \quad \lim_{k \to \infty} \|s_k - s'\|_{\infty} = 0,
\]
and
\[
(s_{k+1}) = (s_k) \pm 2^{k-1} b, \quad \text{for all } i \in [d].
\]
Since the map \(s \mapsto \frac{1}{n} \sum_{i=1}^n Y_{i, b}(s)\) is almost-surely continuous,
\[
\left| \frac{1}{n} \sum_{i=1}^n (Y_{i, b}(s') - Y_{i, b}(s)) 1_{\{X_i \in S_d(\delta)\}} \right| \leq \frac{1}{n} \sum_{k=0}^\infty \left| \frac{1}{n} \sum_{i=1}^n (Y_{i, b}(s_{k+1}) - Y_{i, b}(s_k)) 1_{\{X_i \in S_d(\delta)\}} \right|,
\]
and since \(\sum_{k=0}^\infty \frac{1}{n^{k+1}} \leq 1\), we have the inclusion of events,
\[
\left\{ \sup_{s' \in [-b, b]^d} \left| \frac{1}{n} \sum_{i=1}^n (Y_{i, b}(s') - Y_{i, b}(s)) 1_{\{X_i \in S_d(\delta)\}} \right| \geq a \right\} \subseteq \bigcup_{k=0}^\infty \bigcup_{(s_k) \in \mathcal{H}_k \cap [-b, b]^d} \left\{ \left| \frac{1}{n} \sum_{i=1}^n (Y_{i, b}(s_{k+1}) - Y_{i, b}(s_k)) 1_{\{X_i \in S_d(\delta)\}} \right| \geq \frac{a}{2(k + 1)} \right\}.
By a union bound and the fact that $|H_k \cap [-b, b]^d| \leq 2^{k+2d}$,

$$
(C) \leq \sum_{k=0}^{\infty} 2^{k+2d} \sup_{s_k \in \mathbb{R}^d \cap [-b, b]^d} \sum_{i=1}^{d} P\left( \left| \frac{1}{n} \sum_{j=1}^{n} (Y_{i,b}(s_{k+1}) - Y_{i,b}(s_k)) 1_{\{X_i \in S(b)\}} \right| \geq \frac{a}{2(k+1)^2} \right).
$$

By Azuma’s inequality (see, e.g., Theorem 1.3.1 in [168]), Lemma 4 (Note that $s \in S_{d}(b(d+1))$ and $s' \in s + [-b, b]^d$ imply $s_k \in S_d(b)$ for all $k \in \mathbb{N}_0$, so that

$$
a_1 = \frac{(s_k)}{b} + 1, \ldots, a_d = \frac{(s_k)}{b} + 1, \beta = \frac{1 - \|s\|_1}{b} + 1 \geq 2, \quad \text{for all } k \in \mathbb{N}_0,
$$

and (33), the above is

$$
\leq \sum_{k=0}^{\infty} 2^{k+3d} \cdot 2 \exp \left( -\frac{na^2}{8(k+1)^2} \left( 25d^2 \|f\|_\infty \frac{\|f\|_\infty}{b^{d+1/2} 2^{2k+1}} \right)^2 \right) \leq \sum_{k=0}^{\infty} 2^{k+3d} \cdot 2 \exp \left( -\frac{2^{k-1}}{25d^2 \|f\|_\infty^2} \left( \frac{n^{1/2} d^{d+1/2} a}{\|f\|_\infty \|b\|} \right)^2 \right). \tag{40}
$$

The minimum of $k \mapsto 0.99 \cdot 2^{-k} (k+1)^{-4}$ on $\mathbb{N}_0$ is larger than say $1/16$, so we deduce

$$
(C) \leq C_{f,d} \exp \left( -\frac{1}{100d^2 \|f\|_\infty^2 \|b\|} \cdot \left( \frac{n^{1/2} d^{d+1/2} a}{\|f\|_\infty \|b\|} \right)^2 \right). \tag{41}
$$

for some large constant $C_{f,d} > 0$. Putting (37), (39) and (41) together in (36) concludes the proof of Proposition 1. \hfill \Box

**Corollary 2** (Large deviation estimates). Recall $Y_{i,b}(s)$ from (33). Let $s \in S_{d}(b(d+1))$, $n \geq 100d^6$, $n^{-1/d} \leq b \leq (e^{-16} \sqrt{d} \wedge d^{1/4})$, $0 < a \leq \|f\|_\infty \|b\|/|b^{d+1/2}|$, and take the unique

$$
\delta \in (0, e^{-1}] \quad \text{that satisfies} \quad \delta \log \delta = \frac{b^{d+1/2} a}{\|f\|_\infty \|b\|},
$$

Then, we have

$$
P\left( \sup_{s' \in [-b, b]^d} \left| \frac{1}{n} \sum_{i=1}^{n} Y_{i,b}(s') \right| \geq 2a \right) \leq C_{f,d} \exp \left( -\frac{1}{100d^2 \|f\|_\infty^2 \|b\|} \cdot \left( \frac{n^{1/2} d^{d+1/2} a}{\|f\|_\infty \|b\|} \right)^2 \right), \tag{42}
$$

where $C_{f,d} > 0$ is a constant that depends only on the density $f$ and the dimension $d$.

**Proof of Corollary 2.** By a union bound, the probability in (42) is

$$
P\left( \sup_{s' \in [-b, b]^d} \left| \frac{1}{n} \sum_{i=1}^{n} Y_{i,b}(s') \right| \geq 2a \right) \leq \sup_{s' \in [-b, b]^d} P\left( \left| \frac{1}{n} \sum_{i=1}^{n} Y_{i,b}(s') \right| \geq 2a \right) + \sup_{s' \in [-b, b]^d} P\left( \left| \frac{1}{n} \sum_{i=1}^{n} Y_{i,b}(s') \right| \geq a \right).
$$

The first probability is bounded using Proposition 1. We get the same bound on the second probability by applying Azuma’s inequality and Lemma 4, as we did in (40). \hfill \Box

We are now ready to prove Theorem 4. On the one hand, the Lipschitz continuity of $f$, Jensen’s inequality and (4), imply that, uniformly for $s \in S_{d}$,

$$
f_{s}(s) - f(s) = \mathbb{E}[Y_{i,b}(s)] = \sum_{a \in [d]} \mathcal{O}(\mathbb{E}[|\xi_i - s_i|]) \leq \sum_{a \in [d]} \mathcal{O}(\sqrt{\mathbb{E}[|\xi_i - s_i|^2]}) = \mathcal{O}(b^{1/2}). \tag{43}
$$

On the other hand, recall from (13) that

$$
\hat{f}_{a,b}(s) - f_{b}(s) = \frac{1}{n} \sum_{i=1}^{n} Y_{i,b}(s). \tag{44}
$$

By a union bound over the suprema on hypercubes of width $2b$ centered at each $s \in 2b \mathbb{Z}^d \cap S_{d}(b(d+1))$, and the large deviation estimates in Corollary 2 with

$$
a = 100d^3 \frac{(\log n)^{3/2}}{\sqrt{n}} \cdot \frac{\|f\|_\infty \|b\|}{b^{d+1/2}}. \tag{45}
$$
(the upper bound condition on $a$ is satisfied as long as $100d^2(\log n)^{3/2}/\sqrt{n} \leq e^{-1}$, which is valid if $n \geq 100^6d^6$ for example) and the unique $\delta \in (0, e^{-1}]$ that satisfies

$$\delta \log \delta = \frac{b^{d+1/2}a}{||f||_\infty \log b} \leq 100d^2(\log n)^{3/2}/\sqrt{n},$$

we have

$$\mathbb{P}\left( \sup_{x \in S_{d}(bd)} |\hat{f}_{n,b}(s) - f_b(s)| > 2a \right) \leq \sum_{x \in \mathbb{Z}^d / \mathbb{Z}_d} \mathbb{P}\left( \sup_{x \in [b^{-1} \mathbb{Z}^d]} \frac{1}{n} \sum_{j=1}^{n} Y_{i,b}(s') > 2a \right) \leq b^{-d} \cdot C_{f,d} \exp\left( - \frac{(\log n)^3}{\log \delta} \right).$$

The condition imposed on $\delta$ in (46) implies

$$n^{-1/2} \leq \delta \leq e^{-1},$$

(48)

because the function $x \mapsto x|\log x|$ is increasing on $(0, e^{-1}]$. Using (48) in (47), we get

$$\mathbb{P}\left( \sup_{x \in S_{d}(bd)} |\hat{f}_{n,b}(s) - f_b(s)| > 2a \right) \leq C_{f,d} \exp\left( d \log b - 4 \log n \right).$$

Since we assumed that $b \geq n^{-1/d}$, the above is $\leq C_{f,d} n^{-3}$, which is summable. By our choice of $a$ in (45) and the Borel-Cantelli lemma, we obtain

$$\sup_{x \in S_{d}(bd)} |\hat{f}_{n,b}(s) - f_b(s)| = O(1), \text{ a.s.}$$

Together with (43), the conclusion follows.

6.5. Proof of Theorem 5

By (44), the asymptotic normality of $n^{1/2}b^{d/4}(\hat{f}_{n,b}(s) - f_b(s))$ will be proved if we verify the following Lindeberg condition for double arrays (see, e.g., Section 1.9.3 in [159]): For every $\varepsilon > 0$,

$$n^{-b} \mathbb{E}\left[ |Y_{1,b}(s)|^2 \cdot 1_{|Y_{1,b}(s)| > \varepsilon n^{1/2}b^{d/4}} \right] \rightarrow 0, \quad n \rightarrow \infty,$$

(49)

where $s_b := \mathbb{E}[|Y_{1,b}(s)|^2]$ and $b = b(n) \rightarrow 0$. From Lemma 2, we know that

$$|Y_{1,b}(s)| = O(\psi(s) b^{d/2} \cdot b^{-d}) = O_b(1),$$

and we also know that $s_b = b^{-d/4}\sqrt{\psi(s)f(s)}(1 + o(1))$ when $f$ is Lipschitz continuous, by the proof of Theorem 1, so

$$\frac{|Y_{1,b}(s)|}{n^{1/2}s_b} = O_b(n^{1/2}b^{d/4}b^{-d/2}) = O_b(n^{-1/2}b^{-d/4}) \rightarrow 0,$$

whenever $n^{1/2}b^{d/4} \rightarrow \infty$ as $n \rightarrow \infty$ and $b \rightarrow 0$. Under this condition, (49) holds (since for any given $\varepsilon > 0$, the indicator function is equal to 0 for $n$ large enough, independently of $\omega$) and thus

$$n^{1/2}b^{d/4}(\hat{f}_{n,b}(s) - f_b(s)) = n^{1/2}b^{d/4} \cdot \frac{1}{n} \sum_{i=1}^{n} Y_{i,b,m} \overset{d}{\rightarrow} N(0, \psi(s)f(s)).$$

This ends the proof.

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• F. Ouimet: writing of the original draft and editing, review of the literature, conceptualization, theoretical results and proofs; responsible for Sections 2, 3, 4 and 6, and parts of Section 1.

• R. Tolosana-Delgado: writing of the case study and the practical motivations in the introduction; responsible for Section 5 and parts of Section 1.

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• R. Tolosana-Delgado: writing of the case study and the practical motivations in the introduction; responsible for Section 5 and parts of Section 1.