Nonparametric Estimation of Band-limited Probability Density Functions

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In this paper, a nonparametric maximum likelihood (ML) estimator for band-limited (BL) probability density functions (pdfs) is proposed. The BLML estimator is consistent and computationally efficient. To compute the BLML estimator, three approximate algorithms are presented: a binary quadratic programming (BQP) algorithm for medium scale problems, a Trivial algorithm for large-scale problems that yields a consistent estimator if the underlying pdf is strictly positive and BL, and a fast implementation of the Trivial algorithm that exploits the band-limited assumption and the Nyquist sampling theorem ("BLMLQuick"). All three BLML estimators outperform kernel density estimation (KDE) algorithms (adaptive and higher order KDEs) with respect to the mean integrated squared error for data generated from both BL and infinite-band pdfs. Further, the BLMLQuick estimator is remarkably faster than the KDE algorithms. Finally, the BLML method is applied to estimate the conditional intensity function of a neuronal spike train (point process) recorded from a rat’s entorhinal cortex grid cell, for which it outperforms state-of-the-art estimators used in neuroscience.

probability density | maximum likelihood | band limited | nonparametric | estimation | BLML | BLMLQuick | BLML-BQP | BLMLTrivial

Abbreviations: BLML: Band limited maximum likelihood; pdf: probability density function; KDE: Kernel density estimation; BQP: binary quadratic programming; MISE: mean integrated squared error; MNLL: mean normalized log-likelihood; KDE2nd, KDE6th, KDEsinc: 2nd and 6th order Gaussian and sinc Kernel density estimators; BLMLQuick, BLML-BQP, BLMLTrivial: BLML quick, trivial and BQP algorithms

Significance Statement

Nonparametric estimation of probability densities has become increasingly important to model random phenomena and estimate a pdf. A common approach is to assume that the pdf belongs to a class of parametric functions (e.g., Gaussian, Poisson), and then estimate the parameters by maximizing the data likelihood function. Parametric models have several advantages. First, they are often efficiently computable. Second, the parameters may be related back to physiological and environmental variables. Finally, ML estimates have nice asymptotic properties when the actual distribution lies in the assumed parametric class. However, if the true pdf does not lie in the assumed class of functions, large errors may occur, potentially resulting in misleading inferences.

When little is known a priori about the pdf, nonparametric estimation is an option. However, maximizing the likelihood function yields spurious solutions as the dimensionality of the problem typically grows with the number of data samples, n [1]. To deal with this, several nonparametric approaches penalize the likelihood function by adding a smoothness constraint. Such penalty functions have nice properties of having unique maxima that can be computed. However, when smoothness conditions are applied, the asymptotic properties of ML estimates are typically lost [1].

Other methods for nonparametric estimation assume that the pdf is a linear combination of scaled and stretched versions of a single kernel function [2, 3, 4, 5]. These methods fall under kernel density (KD) estimation, which have been studied for decades. However, choosing an appropriate kernel is still a tricky and often an arbitrary process [6]. Additionally, even the best KD estimators [6, 7, 8, 9] have slower convergence rates (O_p(n^{-4/5}), O_p(n^{-12/13}) for the second and sixth-order Gaussian kernels, respectively) than parametric ML estimation (O_p(n^{-1})) with respect to the mean integrated squared error (MISE) [10].

Finally, some approaches require searching over nonparametric sets for which a maximum likelihood estimate exists. Some cases are discussed in [11, 12], wherein the authors construct maximum likelihood estimators for unknown but Lipschitz continuous pdfs. Although Lipschitz functions display desirable continuity properties, they can be non-differentiable. Therefore, such estimates can be non-smooth, but perhaps more importantly, they are not efficiently computable as a closed-form solution cannot be derived [11, 12].

This paper presents a case where a nonparametric ML estimator exists, is efficiently computable, consistent and results in a smooth pdf. The pdf is assumed to be band-limited (BL), which has a finite-support in the Fourier domain. The BL assumption essentially can be thought of as a smoothness constraint. However, the proposed method does not require penalizing the likelihood function to guarantee the existence of a global maximum, and therefore may preserve the asymptotic properties of ML estimators (i.e. consistency, asymptotic normality and efficiency). The BLML method is first applied to surrogate data generated from both BL and infinite-band pdfs, where in both cases it outperforms all tested KD estimators (including higher order kernels) both in convergence rate and computational time. Then the BLML estimator is applied to the neuronal data recorded from a rat’s entorhinal...
cortex “grid cell” and is shown to outperform state-of-the-art estimators used in neuroscience.

The BLML Estimator. We begin with a description of the BLML estimator in the following theorem.

**Theorem 1.** Consider $n$ independent samples of an unknown BL pdf, $f(x)$, with assumed cut-off frequency $f_c$. Then the BLML estimator of $f(x)$ is given as:

$$
\hat{f}(x) = \left( \frac{1}{n} \sum_{i=1}^{n} \hat{c}_i \sin(\pi f_c(x-x_i)) / \pi (x-x_i) \right)^2,
$$

where $\hat{c} \triangleq [\hat{c}_1, \ldots, \hat{c}_n]^T$ and

$$
\hat{c} = \arg \max_{\rho_n(c) = 0} \left( \prod_{i=1}^{n} \frac{1}{c_i^2} \right).
$$

Here $\rho_n(c) \triangleq \frac{1}{n} \sum_{i=1}^{n} c_j s_{ij} - \frac{n}{c_i^2} \forall i = 1, \ldots, n$ and $s_{ij} \triangleq \frac{\sin(\pi f_c(x_i-x_j))}{\pi (x_i-x_j)} \forall i, j = 1, \ldots, n$.

**Proof:** See supporting information (SI).

The system of equations, $\rho_n(c) = 0$ in (2) is monotonic, i.e., $\frac{\partial \rho_n}{\partial c_i} \geq 0$, with discontinuities at each $c_i = 0$. Therefore, there are $2^n$ solutions, with each solution located in each orthant, identified by the orthant vector $c_0 \triangleq \text{sign}(c)$. Each solution corresponds to a local maximum of the likelihood function which is also its maximum value in that orthant. Hence, the global maximum always exists and can be found by finding the maximum of these $2^n$ maxima. However, it is computationally exhaustive to solve (2), which entails finding the $2^n$ solutions of $\rho_n(c) = 0$ and then comparing values of $\prod_{i=1}^{n} \frac{1}{c_i^2}$ for each solution.

Therefore, to compute the BLML estimator, three approximate algorithms are proposed: a binary quadratic programming (BLML-BQP) algorithm, a BLMLTrivial algorithm, and its quicker implementation - BLMLQuick. Both theory and simulations show that the BLML-BQP algorithm is appropriate when the sample size is $n < 100$ and no additional knowledge is known other than the pdf is BL. However, in cases when $n > 100$ and the underlying pdf is strictly positive, the BLMLTrivial and BLMLQuick algorithms are more appropriate as they are guaranteed to yield a consistent estimate (see Theorems 4, 5 and 6) and converge at a rate ($\sim \frac{1}{n}$), which is faster than all tested KD estimates. Further, the BLMLQuick algorithm shows a remarkable improvement in computational speed over tested KD methods.

Consistency of the BLML Estimator. Proving consistency of the BLML estimator is not trivial as it requires a solution to (2). However, if $f(x) > 0 \ \forall x$ then consistency of BLML estimator can be established. To show this, first an asymptotic solution $\hat{c}_\infty$ to $\rho_n(c) = 0$ is constructed (Theorem 3). Then, consistency is established by plugging $\hat{c}_\infty$ into (1) to show that the ISE and hence the MISE between the resulting density, $f_{\hat{c}}(x)$, and $f(x)$ is 0 (Theorem 4). Then, it is shown that the KL-divergence between $f_{\hat{c}}(x)$ and $f(x)$ is also 0, and hence $\hat{c}_\infty$ is a solution to (2), which makes $f_{\hat{c}}(x)$ the BLML estimator $\hat{f}(x)$ (Theorem 5). Theorems 2-5 and their proofs are presented in SI.

Generalization of the BLML Estimators to Joint Pdfs. Consider the joint pdf $f(x)$, $x \in \mathbb{R}^m$, such that its Fourier transform $F(\omega) \triangleq \int f(x) e^{-j\omega^T \mathbf{x}} dx$ has the element-wise cut off frequencies in vector $\omega_{\text{true}}^{[m]} \triangleq 2\pi k^{[m]}$ true. Then the BLML estimator is of the following form:

$$
\hat{f}(x) = \left( \frac{1}{n} \sum_{i=1}^{n} \hat{c}_i \sin(c_n(x-x_i)) / \pi (x-x_i) \right)^2
$$

where $f_c \in \mathbb{R}^m$ is the assumed cut off frequency, vector $x_i, i = 1 \cdots n$ are the data samples, $\sin(\omega_{\text{true}}^{[m]} x_i) / \pi x_i$ and the vector $\hat{c} \triangleq [\hat{c}_1, \ldots, \hat{c}_n]^T$, is given by

$$
\hat{c} = \arg \max_{\rho_n(c) = 0} \left( \prod_{i=1}^{n} \frac{1}{c_i^2} \right).
$$

Here $\rho_n(c) \triangleq \sum_{i=1}^{n} c_j s_{ij} - \frac{n}{c_i^2}$. $s_{ij} \triangleq \sin(\omega_{\text{true}}^{[m]} x_i - x_j)$.

The multidimensional result can be derived in a very similar way as the one-dimensional result as described in SI.

Computing the BLML Estimator. The three algorithms, BLMLTrivial, BLMLQuick and BLML-BQP are described next.

**BLMLTrivial**

BLMLTrivial is a one-step algorithm that first selects an orthant in which the global maximum may lie, and then solves $\rho_n(c) = 0$ in that orthant. As $\rho_n(c) = 0$ is monotonic, it is computationally efficient to solve in any given orthant.

As stated in Theorem 6 (see SI), the asymptotic solution of (2) lies in the orthant with indicator vector $c_0 = 1 \forall i = 1, \cdots, n$ if $f(x)$ is BL and $f(x) > 0 \ \forall x \in \mathbb{R}$. Therefore, the BLMLTrivial algorithm selects the orthant vector $c_0 = [1, 1, \ldots, 1]^T$ and then $\rho_n(c) = 0$ is solved in that orthant to compute $\hat{c}$. It is important to note that when $f(x)$ is indeed BL and strictly positive, then the BLMLTrivial estimator converges to BLML estimator asymptotically.

Due to its simplicity, the computational complexity of the BLMLTrivial method is very similar to KDE with complexity $O(nl)$, where $l$ is the number of points where the value of pdf is estimated [13]; but the BLMLTrivial method has an extra step of solving equation $\rho_n(c) = 0$. This equation can be solved in $O(n^2)$, using gradient descent or Newton algorithms. Therefore, the computational complexity of BLMLTrivial estimator is $O(n^2 + nl)$.

**BLMLQuick**

The BL assumption of the true pdf allows for a quick implementation of the BLMLTrivial estimator - “BLMLQuick”. For details, see SI. Briefly, BLMLQuick first groups the observed samples into bins of size $< \omega_{\text{true}}^{[m]} / 2$. Then, it constructs the BLMLTrivial estimator of the discrete pdf (or the probability mass function, pmf) that generated the binned data. The true pmf for the binned data has infinite-bandwidth. Hence, under the required conditions, the BLMLTrivial estimate constructed using the Nyquist frequency, $2f_c$, converges to the continuous pdf $f(x)$, from which the pmf is obtained via sampling. $f(x)$ can be made arbitrarily close to the true pdf $f(x)$ by choosing smaller and smaller bins. In fact, if the bin size reduces as $n^{-0.25}$, then the ISE between $f(x)$ and $f(x)$ is of $O(1/n)$. Therefore, the MISE for BLMLQuick is $O(1/n)$ plus the MISE of the BLMLTrivial estimator. Since the MISE of the BLMLTrivial estimator has to be greater than $O(1/n)$, the BLMLQuick algorithm is as efficient as the BLMLTrivial algorithm. Specifically, the computational complexity of BLMLQuick is $O\left(n + f^2_{\text{true}} n^{0.5+2/(r-1)} + f^2 r^{0.25+1/(r-1)} l\right)$, where $\frac{1}{r}$ governs the behavior of the tail of the true pdf.
BLML-BQP Algorithm

To derive the BLML-BQP algorithm, it is first noted that the $2^n$ solutions of $\rho_n(c) = 0$ are equivalent to the $2^n$ local solutions of:

$$\hat{c} = \arg\max_{\epsilon^T \beta \leq n^2} \prod_i \epsilon_i^2. \quad [5]$$

Now, if $c_0 \in \{1,-1\}^n$ is an orthonormal vector and $\lambda \geq 0$ is such that $(A_{c_0})^T S(A_{c_0}) = n^2$, then [5] implies:

$$\prod_i \epsilon_i^2 \geq \lambda^{2^n} = \prod_i \frac{1}{\lambda} \leq \frac{(c_0^T S c_0)^n}{n^{2n}}. \quad [6]$$

Finally, the orthonormal where the solution of [2] lies is found by maximizing the upper bound $\frac{(c_0^T S c_0)^n}{n^{2n}}$ using the following BQP:

$$\hat{c}_0 = \arg\max_{c_0 \in \{1,-1\}^n} (c_0^T S c_0). \quad [7]$$

BQP problems are known to be NP-hard [14], and hence a heuristic algorithm implemented in the gurobi toolbox [15] in MATLAB is used to find an approximate solution $\hat{c}_0$ in polynomial time. Once a reasonable estimate for the orthonormal $\hat{c}_0$ is obtained, $\rho_n(c) = 0$ is solved in that orthonormal to find an estimate for $c$. To further improve the estimate, the solutions to $\rho_n(c) = 0$ in all nearby orthonormals (Hamming distance equal to one) of the orthonormal $\hat{c}_0$ are obtained and subsequently $\frac{1}{\epsilon_i^2}$ is evaluated in these orthonormals. The neighboring orthonormal with the largest $\frac{1}{\epsilon_i^2}$ is set as $c_0$, and the process was repeated. This iterative process is continued until $\frac{1}{\epsilon_i^2}$ for all nearby orthonormals is no greater than that of the current orthonormal. The BLML-BQP is computationally expensive, with complexity $O(n^2 + n! + BQP(n))$ where $BQP(n)$ is the computational complexity of solving BQP problem of size $n$. Hence, the BLML-BQP algorithm can only be used on data samples $n < 100$.

Results

A comparison of BLMLTrivial and BLML-BQP algorithms on surrogate data generated from known pdfs is presented first. Then, the performance of the BLMLTrivial and BLMLQuick algorithms is compared to several KD estimators. Finally, we show the application results of BLML, KD and GLM methods to neuronal spiking data.

Performance of BLMLTrivial versus BLML-BQP on Surrogate Data. In Figure 1, BLMLTrivial and BLML-BQP estimates are presented assuming that the true pdfs are BL by $f_c = f_c^{true}$. In Figure 2, we compare the results of the BLMLTrivial and BLMLQuick estimators to the KDE2nd, KDE6th and sinc KD estimators. Comparison of the MISE as a function of $n$ for (A) a strictly positive band-limited true pdf (the one used in Figure 1B) and (B) an infinite band Gaussian normal pdf. For the BLML estimators the cut-off frequencies are chosen as $f_c = 2f_c^{true}$ for the BL true pdf and $f_c = 2$ for the normal true pdf. For the KDE2nd and KDE6th, the optimal bandwidths were chosen as $q = 0.6n^{-0.2}$ and $0.6n^{-1/3}$, respectively, and also to match the MISE for the BLML estimator for $n = 1$. For the KDESinc, the $f_c$ was kept the same as the $f_c$ for BLML estimators. (C) The MISE as a function of the cutoff frequency $\frac{1}{f_c}$ for a BL true pdf with cut-off frequency $f_c^{true}$. $n = 10^4$ was used for creating this plot. (D) Computation time as a function of $n$. The p-values were calculated between the BLMLTrivial estimator and other estimators using paired t-tests for either $\log_{10}(n) = 5$ (A,B,D) or $\log_{10}(f_c/f_c^{true}) = 1.6$ (C) and are color coded.
Panels (A, C) and (B, D) use surrogate data generated from a non-strictly positive pdf \( f_x = 0.4 \sin^2(0.4x) \) and strictly positive pdf \( f(x) = \frac{3x^2}{4} \sin^2(0.2x) + \sin^2(0.2x + 0.1) \), respectively. Both pdfs are BL from \((-0.4, 0.4)\). In Panels A and B, the BLML estimates (\( n = 81 \)) are plotted using both algorithms, and the true pdfs are overlayed for comparison. In Panels C and D, the MISE is plotted as a function of sample size \( n \) for both algorithms and both pdfs. For each \( n \), data were generated 100 times to generate 100 estimates from each algorithm. The mean of the ISE was then taken over these 100 estimates to generate the MISE plots.

As expected from theory, the **BLML-BQP** algorithm works best for the non-strictly positive pdf, whereas the **BLMLTrivial** algorithm is marginally better for the strictly positive pdf. Note that as \( n \) increases beyond 100, the **BLML-BQP** algorithm becomes computationally expensive, therefore the **BLMLTrivial** and **BLMLQuick** algorithms are used in the remainder of this paper with the assumption that the true pdf is strictly positive.

**BLML and KDE on Surrogate Data.** The performance of the **BLMLTrivial** and **BLMLQuick** estimates is compared with adaptive KD estimators which are the fastest known non-parametric estimators with convergence rates of \( O(n^{-3/5}) \), \( O(n^{-12/13}) \) and \( O(n^{-4}) \) for 2nd-order Gaussian (KDE2nd), 6th-order Gaussian (KDE6th) and sinc (KDESinc) kernels, respectively [16, 18]. Panels A and B of Figure 2 plot the MISE of the BLML estimators using the **BLMLTrivial**, **BLMLQuick**, and the adaptive KD approaches for cases in the presence of BL or non-BL pdf, respectively. In the BL case, the true pdf is strictly positive and is the same as used above, and for the infinite-band case, the true pdf is normal. For the **BLMLTrivial**, **BLMLQuick** and sinc KD estimates, \( f_2 = 2f_{true} \) and \( f_x = 2 \) are used for the BL and infinite-band cases, respectively. For the 2nd and 6th-order KD estimates, the optimal bandwidths \((q = \frac{1}{8}n^{-1/5} \) and \( q = \frac{9}{2}n^{-1/13} \) respectively) are used. The constant \( \frac{4}{7} \) ensures that MISEs are matched for \( n = 1 \).

It can be seen from the Figure that for both the BL and infinite-band cases, **BLMLTrivial** and **BLMLQuick** outperform KD methods. In addition, the BLML estimators seem to achieve a convergence rate that is as fast as the KDESinc, which is known to have a convergence rate of \( O(n^{-4}) \). Figure 2C plots the MISE as a function of the cut-off frequency \( f_{true} \) for the BL pdf. **BLMLTrivial** and **BLMLQuick** seem to be most sensitive to the correct knowledge of \( f_x \), as it shows larger errors when \( f_x < f_{true} \), which quickly dip as \( f_x \) approaches \( f_{true} \). When \( f_x > f_{true} \), the MISE increases linearly and the BLML methods have smaller MISEs as compared to KD methods.

Finally, Figure 2D plots the computational time of the BLML and KD estimators. All algorithms were implemented in MATLAB, and in-built MATLAB 2013a algorithms were used to compute the 2nd and 6th-order adaptive Gaussian KD and sinc KD estimators. The results concur with theory and illustrate that **BLMLTrivial** is slower than KD approaches for large number of observations, however, the **BLMLQuick** algorithm is remarkably quicker than all KD approaches and **BLMLTrivial** for both small and large \( n \).

**BLML Applied to Neuronal Spiking Data.** Neurons generate action potentials in response to external stimuli and intrinsic factors, including the activity of its neighbors. The sequence of action potentials over time can be abstracted as a point process, where the timing of action potentials or “spikes” carry important information. The stochastic point process is characterized by a conditional intensity function (CIF), denoted as \( \lambda(\cdot) \).

Here, the BLML, KD, and GLM methods are applied to estimate the CIF of a “grid cell” from spike train data. In the experimental set up, the Long-Evans rat was freely foraging in an open field arena of radius of 1m for a period of 30-60 minutes. Custom microelectrode drives with variable numbers of tetrodes were implanted in the rat’s medial entorhinal cortex and dorsal hippocampal CA1 area. Spikes were acquired with a sampling rate of 31.25 kHz and filter settings of 300 Hz-6 kHz. Two infrared diodes alternating at 60 Hz were attached to the drive of each animal for position tracking. Spike sorting was accomplished using a custom manual clustering program (Xclust, M.A. Wilson). All procedures were approved by the MIT Institutional Animal Care and Use Committee.

The spiking activity of grid cell is known to be phase-modulated, whose peak firing locations define a grid-like array covering much of the 2-dimensional arena. A spike histogram of the selected cell as a function of the rat’s position is shown in Figure 3A, which plots the \((x, y)\) coordinates of the rat’s position when the cell generate spikes (red dots) and the rat’s trajectory inside the arena (blue trajectory). The CIF was then estimated as a function of the rat’s position (stimuli) and the neuron’s spiking history (intrinsic factors):

\[
\lambda(t|x, y, h) \triangleq \lim_{\Delta t \to 0} \frac{\mathbb{P} \text{spike in time } \Delta t | x, y, h, x_{t}, y_{t} = (x, y)}{\Delta t}
\]

where \( x(t), y(t) \) is the rat’s position over time inside an arena, and the vector \( H_t \), consists of spiking history covariates at time \( t \) as in [18, 19, 20, 21, 22].

Baye’s rule [23] allows one to use nonparametric approaches to estimate \( \lambda(\cdot) \) as follows [24]:

\[
\lambda(t|x, y, h) \approx \frac{N}{T} \frac{f(x, y, h)}{f(x, y, h) | \text{spike in time } \Delta t}
\]

where \( h(t) \triangleq \log(\text{time since last spike}) \), \( N \) is the total number of spikes within time interval \( T \), which is the total duration of the spike train observation. \( f(x, y, h) \) and \( f(x, y, h) | \text{spike in time } \Delta t \) are densities which are estimated using both KDE2nd (higher order kernels were too slow for estimation) and **BLMLQuick** methods. The use of the logarithm allows for a smoother dependence of \( \lambda \) on \( h \), which in turn allows for capturing high frequency components in the CIF due to refractoriness (i.e., sharp decrease in \( \lambda(t) \) after a spike) and bursting.

The bandwidths and cut-off frequencies used are \( q_x = q_y = 0.5n^{-0.2} \), \( q_x = 0.5n^{-0.2} \) and \( f_x = f_y = 1.4 \), \( f_y = 1.75 \) for KDE2nd and **BLMLQuick** respectively. These bandwidths and cut-off frequencies were chosen after testing different combinations, and the frequencies and bandwidths that best fits the test data (i.e., had the lowest KS statistics, see below) for each method were used. Since the rat cannot leave the circular arena, the estimates \( f(x, y, h) | \text{spike in time } \Delta t \) and \( f(x, y, h) \) are normalized to integrate to 1 within the arena. The nonparametric estimates of \( \lambda \) are also compared with two popular GLMs:

1. Gaussian GLM (GLMgauss)

\[
\log(\lambda(x, y, H)) = \alpha_1 + \alpha_2 x + \alpha_3 y + \alpha_4 x^2 + \alpha_5 y^2 + \alpha_6 xy + \sum_{i=1}^{25} \beta_i h_i
\]

2. Zernike GLM (GLMzern)

\[
\log(\lambda(x, y, H)) = \sum_{i,j} \gamma_{i,j} \chi(i, j) + \sum_{i=1}^{25} \beta_i h_i
\]

where \( \alpha_1, \ldots, \alpha_6, \beta_i, \gamma_{i,j} \) are the parameters estimated from the data. \( H \triangleq [h_1, \ldots, h_{25}]^T \) where \( h_i \) are the number of
spikes in \((t - 2i, t - 2i + 2) ms\) and \(\chi(i, j)\) are Zernike polynomials of 3rd order.

The goodness-of-fit of the four estimates of \(\lambda\) are computed using the time rescaling theorem and the Kolmogorov-Smirnov (KS) statistic [25]. Briefly, 80% of the data is used to estimate \(\lambda\) and then the empirical CDF of rescaled spike times is computed using the remaining 20% test data, which should follow a uniform CDF if the estimate of \(\lambda\) is accurate.

The similarity between the two CDFs is quantified using the Kolmogorov-Smirnov (KS) statistic [25]. Briefly, 80% of the data is used to estimate \(\lambda\) and then the empirical CDF of rescaled spike times is computed using the remaining 20% test data, which should follow a uniform CDF if the estimate of \(\lambda\) is accurate.

The KS-plot for BLMLTrivial (blue), KDE2nd (purple), GLM Gaussian (black) and GLM Zernike (red), along with 95% confidence intervals (dashed lines) using 20% of test data. (c) Estimated \(\lambda(t)\) using the four methods. All four methods show refractoriness and bursting.

Discussion

In this paper, a nonparametric ML estimator for BL densities is developed and its consistency is proved. In addition, three heuristic algorithms that allow for quick computation of the BLML estimator are presented. Although these algorithms are not guaranteed to generate the BLML estimate, we show that for strictly positive pdfs, the BLMLTrivial and BLMLQuick estimates converge to the BLML estimate asymptotically. Further, BLMLQuick is remarkably quicker than all tested KD methods, while maintaining convergence rates of BLML estimators. Even further, using surrogate data, it is shown that both the BLMLTrivial and BLMLQuick estimators have an apparent convergence rate of \(1/n\) for MISE, which is equal to that of parametric methods. Finally, BLML is applied to spiking data, where it outperforms state-of-the-art estimation techniques used in neuroscience.

The BLML estimators may be motivated by quantum mechanics. The function \(g(x)\) in the development of BLML estimate (see SI) is analogous to the wave function [26] in quantum mechanics, where the square of the absolute value of both are probability density functions. In addition, in quantum mechanics the wave function of momentum is the Fourier transform of the wave function of position. Therefore, if the momentum wave function has finite support, then the position wave function is BL and vice versa. Such occurrences are frequent in the single or double slit experiment, where one observes bandlimited (\(\sin^2(f_1x)\) and \(\cos^2(f_2x)\) respectively) profile for the probability of finding a particle at a distance \(x\) from the center. Also, in the thought experiment of a particle in a box: the wave function for position has finite support, making the momentum wave function BL. We suspect that a large number pdfs in the nature are BL because macro world phenomena are a sum of quantum level phenomenon and pdf at quantum level are shown to be BL (single and double slit experiments). Furthermore, the set of BL pdfs is complete, i.e. the sum of two random variables that each have a BL pdf is a random variable whose pdf is a convolution of original pdfs, and hence is BL. Therefore, if macro level phenomenon is a linear combination of different quantum level phenomenon with BL pdfs, then the macro level phenomenon will also gen-
erate a BL pdf. In fact, we see this at macro level where we observe Gaussian pdfs of various processes. The Gaussian pdf is almost BL, with cutoff frequency \( f_c = 1/\sigma \) (< \( 10^{-24} \) GHz of its power lies outside this band). In fact, given finite data, it is impossible to distinguish if the data is generated by a Gaussian or BL pdf.

**Choosing A Cut-off Frequency for the BLML Estimator.** The BLML method requires selecting a cut-off frequency of the unknown pdf. One strategy for estimating the true cut-off frequency is to first fit a Gaussian pdf using the data via ML estimation. Once an estimate for standard deviation is obtained, one can estimate the cut-off frequency using the formula \( f_c = 1/\sigma \), as this will allow most power of the true pdf to lie within the assumed band if the true pdf has Gaussian-like tails.

Another strategy is to increase the assumed cut-off frequency of BLML estimator as a function of the sample size. For such a strategy, the BLML estimator may converge even when the true pdf has an infinite frequency band, provided that the increase in cut-off frequency is slow enough and the cut-off frequency approaches infinity asymptotically, e.g. \( \omega_n \propto \log(n) \).

A more sophisticated strategy would be to look at the mean normalized log-likelihood (MNLL), \( \mathbb{E}(\mathcal{N} \sum \log(c_i^2)) \) as a function of assumed cut-off frequency \( f_c \). Figure 4 plots MNLL (calculated using BLMLTrivial algorithm) is plotted for \( n = 200 \) samples from a strictly positive true pdf \( f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \) along with \( \frac{\partial^2 \text{MNLL}}{\partial f_c^2} \). Note that \( \frac{\partial^2 \text{MNLL}}{\partial f_c^2} \approx \mathbb{E}(\sum_{ij} c_i^2 c_j^2) \), where \( c_i \triangleq \cos(f_c(x_i - x_j)) \).

We see that the MNLL rapidly increases until \( f_c \) reaches \( f_c^{\text{true}} \), after which the rate of increase sharply declines. There is a clear “knee” in both MNLL and \( \frac{\partial^2 \text{MNLL}}{\partial f_c^2} \) curves at \( f_c = f_c^{\text{true}} \). Therefore, \( f_c^{\text{true}} \) can be inferred from such a plot. A more complete mathematical analysis of this “knee” is left for future work.

**Making BLMLQuick Even Faster.** There are several faster implementation of KD approaches such as those presented in [16, 27]. These approaches use numerical techniques to evaluate the sum of \( n \) kernels over \( f \) given points. Such techniques may also be incorporated while calibrating the BLMLQuick estimator to make it even faster. Exploration of this idea will be done in a future study.

**Asymptotic Properties of the BLML Estimator.** Although, this paper proves that the BLML estimate is consistent, it is not clear whether it is asymptotically normal and efficient (i.e., achieving a Cramer-Rao-like bound). Studying asymptotic normality and efficiency is nontrivial for BLML estimators as one would need to first redefine asymptotic normality and extend the concepts of Fisher information and the Cramer-Rao lower bound to the nonparametric case. Therefore, we leave this to a future study. However, we postulate here that the curvature of MNLL plot might be related to Fisher information in the BLML case. In addition, although under simulations, the BLML estimator seems to achieve a convergence rate similar to its parametric counterparts (\( O_p(n^{-1}) \)) it is not proved theoretically.

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