A complex exponential Fourier transform approach to gradient density estimation

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Abstract

We prove a novel result wherein the density function of the gradients of a thrice differentiable function S (obtained via a random variable transformation of a uniformly distributed random variable) defined on a closed, bounded interval $\Omega \subset \mathbb{R}$ is accurately approximated by the normalized power spectrum of $\phi = \exp\left(\frac{iS}{\tau}\right)$ as the free parameter $\tau \to 0$. The result is shown using the well known stationary phase approximation and standard integration techniques and requires proper ordering of limits. Experimental results provide anecdotal visual evidence corroborating the result.

1. Introduction

The literature is replete with techniques which attempt to estimate a non-observable probability density function using observed data believed to be sampled from an underlying distribution. Density estimation techniques have a long history and run the gamut of histogramming, Parzen windows [see Parzen (1962)], vector quantization, wavelets etc. In the present work, we prove a novel mathematical result relating the density function of the gradients of a function S [viewed as a random variable transformation $Y = S'(X)$ where X is uniformly distributed] with the normalized power spectrum of $\exp\left(\frac{iS}{\tau}\right)$ as the quantity $\tau \to 0$.

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We provide a simple Fourier transform-based technique to determine the density of Y. Our method computes the gradient density directly from the function S, circumventing the need to compute its derivative S'. The approach is based on expressing the function S as the phase of a wave function ϕ, specifically $\phi(x) = \exp\left(\frac{iS(x)}{\tau}\right)$ for small values of τ and then considering the normalized power spectrum—magnitude squared of the Fourier transform of ϕ [see Bracewell (1999)]. Using the *stationary phase approximation*—a well known technique in asymptotic analysis [please see Olver (1974a)]—we show that in the limiting case as $\tau \to 0$, the power spectrum of ϕ converges to the density of Y and hence can serve as its density estimator at small, non-zero values of τ.

Our new mathematical relationship is motivated by the classical-quantum relation, wherein classical physics is expressed as a limiting case of quantum mechanics [please refer to Griffiths (2004); Feynman and Hibbs (1965)]. When S is treated as the Hamilton-Jacobi scalar field, the gradient of S corresponds to the classical momentum of a particle [see Goldstein et al. (2001)]. In the parlance of quantum mechanics, the magnitude square of the wave function expressed either in its position or momentum basis corresponds to its position or momentum density respectively. Since these representations (either in the position or momentum basis) are simply the (suitably scaled) Fourier transforms of each other, the magnitude square of the Fourier transform of the wave function expressed in its position basis, is its quantum momentum density [see Griffiths (2004)]. The principal theorem proved in the article [Theorem (2.5)] states that the classical momentum density (denoted by P) can be expressed as a limiting case (as $\tau \to 0$) of its corresponding quantum momentum density (denoted by P_τ), in complete agreement with the correspondence principle [see Griffiths (2004)].

2. Equivalence of the gradient density and the power spectrum

As stated above, the density function for the gradients of S (denoted by Y) can be obtained via a random variable transformation of a uniformly distributed random variable X using the derivative S' as the transformation function, namely, $Y = S'(X)$. We assume that S is thrice differentiable on a closed, bounded interval $\Omega = [b_1, b_2]$ (with length $L = b_2 - b_1$) and has a non-vanishing second derivative *almost everywhere*

on Ω, i.e.

$$\mu\left(\{x : S''(x) = 0\}\right) = 0, \tag{2.1}$$

where μ denotes the Lebesgue measure. The assumption in (2.1) is made in order to ensure that the density function of Y exists almost everywhere. This is further clarified in Lemma 2.2 below.

Define the following sets:

$$
\begin{aligned}
\mathcal{B} &\equiv \{x : S''(x) = 0\}, \\
\mathcal{C} &\equiv \{S'(x) : x \in \mathcal{B}\} \cup \{S'(b_1), S'(b_2)\}, \text{ and} \\
\mathcal{A}_u &\equiv \{x : S'(x) = u\}. \tag{2.2}
\end{aligned}
$$

Here, $S'(b_1) = \lim_{x \to b_1^+} S'(x)$ and $S'(b_2) = \lim_{x \to b_2^-} S'(x)$. The higher derivatives of S at the end points b_1, b_2 are also defined along similar lines using one-sided limits. The main purpose of defining these one-sided limits is to exactly determine the set $\mathcal{C}$ where the density of Y is *not defined*. Since $\mu(\mathcal{B}) = 0$, we also have $\mu(\mathcal{C}) = 0$.

Lemma 2.1. *[Finiteness Lemma] $\mathcal{A}_u$ is finite for every $u \notin \mathcal{C}$.*

Lemma 2.2. *[Density Lemma] The probability density of Y on $\mathbb{R} - \mathcal{C}$ exists and is given by*

$$P(u_0) = \frac{1}{L} \sum_{k=1}^{N(u_0)} \frac{1}{|S''(x_k)|}, \tag{2.3}$$

where the summation is over $\mathcal{A}_{u_0}$ (which is the finite set of locations $x_k \in \Omega$ where $S'(x_k) = u_0$ as per Lemma 2.1), with $|\mathcal{A}_{u_0}| = N(u_0)$.

Since the density is based on the transformation $Y = S'(X)$, the probability density function in (2.3) assumes the existence of the inverse of the transformation function S' [see Billingsley (1995)]. This is made explicit in the following lemma which is required by the main theorem.

Lemma 2.3. *[Interval Lemma] For every $u \notin \mathcal{C}$, $\exists \eta > 0$ and a closed interval $\mathcal{J}_\eta = [u - \eta, u + \eta]$ such that $\mathcal{J}_\eta \cap \mathcal{C}$ is empty.*

The proofs of the lemmas are available in AppendixA.

We now prove the main result which relates the normalized power spectrum of $\exp\left(\frac{iS(x)}{\tau}\right)$ (in the limit as $\tau \to 0$) with the probability density of the random variable $Y = S'(X)$ (denoted by P).

Define a function $F : \mathbb{R} \times \mathbb{R}^+ \to \mathbb{C}$ as

$$F(u, \tau) \equiv \frac{1}{\sqrt{2\pi\tau L}} \int_{b_1}^{b_2} \exp\left(\frac{iS(x)}{\tau}\right) \exp\left(\frac{-iux}{\tau}\right) dx. \qquad (2.4)$$

For a fixed value of τ, define a function $F_\tau : \mathbb{R} \to \mathbb{C}$ as

$$F_\tau(u) \equiv F(u, \tau). \qquad (2.5)$$

Observe that F_τ is closely related to the Fourier transform of $\exp\left(\frac{iS(x)}{\tau}\right)$. The scale factor $\frac{1}{\sqrt{2\pi\tau L}}$ is the normalizing term such that the L_2 norm of F_τ is one as seen in the following lemma (whose proof is straightforward and omitted for lack of space).

Lemma 2.4. *With F_τ defined as above, $F_\tau \in L^2(\mathbb{R})$ and $\|F_\tau\| = 1$.*

Define a function $P_\tau : \mathbb{R} - \mathcal{C} \to \mathbb{R}^+$ as

$$P_\tau(u) \equiv |F_\tau(u)|^2 = F_\tau(u)\overline{F_\tau(u)}. \qquad (2.6)$$

By definition, $P_\tau \geq 0$. Since $\mu(\mathcal{C}) = 0$, from Lemma (2.4), $\int_{-\infty}^{\infty} P_\tau(u)du = 1$. Hence, treating $P_\tau(u)$ as a density function, we have the following theorem statement.

Theorem 2.5. *If P and P_τ are defined as above, then the*

$$\lim_{\alpha \to 0} \frac{1}{\alpha} \lim_{\tau \to 0} \int_{u_0}^{u_0+\alpha} P_\tau(u)du = P(u_0), \ \forall u_0 \notin \mathcal{C}. \qquad (2.7)$$

Before embarking on the proof, we would like to emphasize that the ordering of the limits and the integral as given in the theorem statement is crucial and cannot be arbitrarily interchanged. To press this point home, we show below that after solving for P_τ, the $\lim_{\tau \to 0} P_\tau$ does not exist. Hence, the order of the integral followed by the limit $\tau \to 0$ cannot be interchanged. Furthermore, when we swap the limits between α and τ, we get

$$\lim_{\tau \to 0} \lim_{\alpha \to 0} \frac{1}{\alpha} \int_{u_0}^{u_0+\alpha} P_\tau(u)du = \lim_{\tau \to 0} P_\tau(u_0) \qquad (2.8)$$

which does not exist. Hence, the theorem statement can be valid *only* for the specified sequence of limits and the integral.

2.1. Brief exposition of the result

To understand the result in simpler terms, let us reconsider the definition of the scaled Fourier transform given in (2.4). The first exponential $\exp\left(\frac{iS}{\tau}\right)$ is a varying complex "sinusoid", whereas the second exponential $\exp\left(\frac{-iux}{\tau}\right)$ is a fixed complex sinusoid at frequency $\frac{u}{\tau}$. When we multiply these two complex exponentials, at low values of τ, the two sinusoids are usually not "in sync" and tend to cancel each other out. However, around the locations where $S'(x) = u$, the two sinusoids are in perfect sync (as the combined exponent is *stationary*) with the approximate duration of this resonance depending on $S''(x)$. The value of the integral in (2.4) can be approximated via the stationary phase approximation [please see Olver (1974a)] as

$$F_\tau(u) \approx \frac{1}{\sqrt{L}} \exp\left(\pm i \frac{\pi}{4}\right) \sum_{k=1}^{N(u)} \exp\left\{\frac{i}{\tau}\left(S(x_k) - ux_k\right)\right\} \frac{1}{\sqrt{S''(x_k)}} \qquad (2.9)$$

where $N(u) = |\mathcal{A}_u|$. The approximation is increasingly tight as $\tau \to 0$. The squared Fourier transform (P_τ) gives us the required result $\frac{1}{L}\sum_{k=1}^{N(u)} \frac{1}{|S''(x_k)|}$ except for the *cross* phase factors $S(x_k) - S(x_l) - u(x_k - x_l)$ obtained as a byproduct of two or more remote locations x_k and x_l indexing into the same frequency bin u, i.e, $x_k \neq x_l$, but $S'(x_k) = S'(x_l) = u$. Integrating the squared Fourier transform over a small frequency range $[u, u + \alpha]$ removes these cross phase factors and we obtain the desired result.

2.2. Formal proof

We shall now provide the proof by considering different cases.

case (i): Let us consider the case in which no stationary points exist for the given u_0, i.e, there is no $x \in \Omega$ for which $S'(x) = u_0$. Let $t(x) = S(x) - u_0 x$. Then, $t'(x)$ is of constant sign in $[b_1, b_2]$ and hence $t(x)$ is strictly monotonic. Defining $v = t(x)$, we have from (2.4),

$$F_\tau(u_0) = \frac{1}{\sqrt{2\pi\tau L}} \int_{t(b_1)}^{t(b_2)} \exp\left(\frac{iv}{\tau}\right) g(v) dv. \qquad (2.10)$$

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Here, $g(v) = \frac{1}{t'(x)}$ where $x = t^{-1}(v)$. Integrating by parts, we get

$$
\begin{aligned}
F_\tau(u_0)\sqrt{2\pi\tau L} &= \frac{\tau}{i}\left[\exp\left(\frac{it(b_2)}{\tau}\right)g\left(t(b_2)\right) - \exp\left(\frac{it(b_1)}{\tau}\right)g\left(t(b_1)\right)\right] \\
&\quad -\frac{\tau}{i}\int_{t(b_1)}^{t(b_2)}\exp\left(\frac{iv}{\tau}\right)g'(v)dv.
\end{aligned}
\tag{2.11}
$$

Then

$$
|F_\tau(u_0)|\sqrt{2\pi\tau L} \leq \tau\left(\frac{1}{|S'(b_2) - u_0|} + \frac{1}{|S'(b_1) - u_0|} + \int_{t(b_1)}^{t(b_2)}|g'(v)|\,dv\right).
\tag{2.12}
$$

Hence, $|F_\tau(u_0)| \leq \gamma_1(u_0)\sqrt{\tau}$, where $\gamma_1(u_0) > 0$ is a continuous function of u_0. Then $P_\tau(u_0) \leq \gamma_1^2(u_0)\tau$. Since $S'(x)$ is continuous and $u_0 \notin \mathcal{C}$, we can find a $\rho > 0$ such that for every $u \in [u_0 - \rho, u_0 + \rho]$, no stationary points exist. The value ρ can also be chosen appropriately such that $[u_0 - \rho, u_0 + \rho] \cap \mathcal{C} = \emptyset$. If $|\alpha| < \rho$, then

$$
\lim_{\tau \to 0}\int_{u_0}^{u_0 + \alpha}P_\tau(u)du = 0.
\tag{2.13}
$$

Furthermore, from (2.3) we have $P(u_0) = 0$. The result immediately follows.

case (ii): We now consider the case where stationary points exist. Since we are interested only in the situation as $\tau \to 0$, the stationary phase method in Olver (1974a,b) can be used to obtain a good approximation for $F_\tau(u_0)$ defined in (2.4) and (2.5). The phase term in this function, $\frac{S(x) - u_0 x}{\tau}$, is stationary only when $S'(x) = u_0$. Consider the set $\mathcal{A}_{u_0}$ defined in (2.2). Since it is finite by Lemma (2.1), let $\mathcal{A}_{u_0} = \{x_1, x_2, \ldots, x_{N(u_0)}\}$ with $x_k < x_{k+1}, \forall k$. We break Ω into disjoint intervals such that each interval has utmost one stationary point. To this end, consider numbers $\{c_1, c_2, \ldots, c_{N(u_0)+1}\}$ such that $b_1 < c_1 < x_1$, $x_k < c_{k+1} < x_{k+1}$ and $x_{N(u_0)} < c_{N(u_0)+1} < b_2$. Let $t(x) = S(x) - u_0 x$. Then,

$$
F_\tau(u_0)\sqrt{2\pi\tau L} = G_1 + G_2 + \sum_{k=1}^{N(u_0)}(K_k + \tilde{K}_k)
\tag{2.14}
$$

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where

$$G_1 = \int_{b_1}^{c_1} \exp\left(\frac{it(x)}{\tau}\right) dx,$$

$$G_2 = \int_{c_{N(u_0)+1}}^{b_2} \exp\left(\frac{it(x)}{\tau}\right) dx,$$

$$K_k = \int_{c_k}^{x_k} \exp\left(\frac{it(x)}{\tau}\right) dx, \text{ and}$$

$$\tilde{K}_k = \int_{x_k}^{c_{k+1}} \exp\left(\frac{it(x)}{\tau}\right) dx. \qquad (2.15)$$

Note that the integrals G_1 and G_2 do not have any stationary points. From case (i) above, we get

$$G_1 + G_2 = \epsilon_1(u_0, \tau) = O(\tau) \qquad (2.16)$$

as $\tau \to 0$. Furthermore, $\epsilon_1(u_0, \tau) \le \gamma_2(u_0)\tau$, where $\gamma_2(u_0) > 0$ is a continuous function of u_0. In order to evaluate K_k and $\tilde{K}_k$, observe that when we expand the phase term up to second order, $t(x) - t(x_k) \to Q(x_k)(x - x_k)^2$ as $x \to x_k$, where $Q(x_k) = \frac{S''(x_k)}{2}$. Furthermore, in the open intervals (c_k, x_k) and (x_k, c_{k+1}), $t'(x) = S'(x) - u_0$ is continuous and is of constant sign. From Theorem 13.1 in Olver (1974a), we get

$$\tilde{K}_k = K_k = \frac{1}{2}\exp\left(\pm\frac{i\pi}{4}\right)\Gamma\left(\frac{1}{2}\right)\exp\left(\frac{it(x_k)}{\tau}\right)\sqrt{\frac{2\tau}{|S''(x_k)|}} + \epsilon_2(u_0, \tau). \quad (2.17)$$

From Lemma 12.3 in Olver (1974a), it can be verified that $\epsilon_2(u_0, \tau) = o(\sqrt{\tau})$ as $\tau \to 0$ and can also be *uniformly bounded* by a function of u_0 (independent of τ) for small values of τ. In (2.17), Γ is the Gamma function and the sign in the phase term depends on whether $S''(x_k) > 0$ or $S''(x_k) < 0$. Plugging the values of these integrals in (2.14) and noting that $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$, we get

$$F_\tau(u_0)\sqrt{2\pi\tau L} = \sum_{k=1}^{N(u_0)} \exp\left(\frac{i}{\tau}[S(x_k) - u_0 x_k]\right)\sqrt{\frac{2\pi\tau}{|S''(x_k)|}}\exp\left(\pm\frac{i\pi}{4}\right)$$
$$+ \epsilon_1(u_0, \tau) + \epsilon_2(u_0, \tau). \qquad (2.18)$$

Hence,

$$F_\tau(u_0) = \frac{1}{\sqrt{L}}\sum_{k=1}^{N(u_0)} \frac{\exp\left(\frac{i}{\tau}[S(x_k) - u_0 x_k]\right)}{\sqrt{|S''(x_k)|}}\exp\left(\pm\frac{i\pi}{4}\right) \qquad (2.19)$$
$$+ \epsilon_3(u_0, \tau), \qquad (2.20)$$

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where $\epsilon_3(u_0, \tau) = \frac{\epsilon_1(u_0,\tau)+\epsilon_2(u_0,\tau)}{\sqrt{2\pi\tau L}} = o(1)$ as $\tau \to 0$.

From the definition of $P_\tau(u)$ in (2.6), we have

$$
\begin{aligned}
P_\tau(u_0) \quad = \quad & \frac{1}{L} \sum_{k=1}^{N(u_0)} \frac{1}{|S''(x_k)|} \\
& + \frac{1}{L} \sum_{k=1}^{N(u_0)} \sum_{l=1; l \neq k}^{N(u_0)} \frac{\cos\left(\frac{1}{\tau}[S(x_k) - S(x_l) - u_0(x_k - x_l)] + \theta(x_k, x_l)\right)}{|S''(x_k)|^{\frac{1}{2}} |S''(x_l)|^{\frac{1}{2}}} \\
& + \epsilon_4(u_0, \tau), \quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad (2.21)
\end{aligned}
$$

where $\epsilon_4(u_0, \tau)$ includes both the magnitude square of $\epsilon_3(u_0, \tau)$ and the cross terms involving the main (first) term in (2.19) and $\epsilon_3(u_0, \tau)$. Notice that the main term in (2.19) can be bounded by a function of u_0 *independent* of τ as

$$
\left| \exp\left(\frac{i}{\tau}[S(x_k) - u_0 x_k]\right) \right| = 1, \forall \tau \quad\quad\quad\quad (2.22)
$$

and $S''(x_k) \neq 0, \forall k$. Since $\epsilon_3(u_0, \tau) = o(1)$, we get $\epsilon_4(u_0, \tau) = o(1)$ as $\tau \to 0$. Additionally, $\theta(x_k, x_l) = 0, \frac{\pi}{2}$ (or $-\frac{\pi}{2}$) and $\theta(x_l, x_k) = -\theta(x_k, x_l)$.

The first term in (2.21) exactly matches the expression for $P(u_0)$ as seen from Lemma (2.2). But, since $\lim_{\tau \to 0} \cos\left(\frac{1}{\tau}\right)$ is not defined, $\lim_{\tau \to 0} P_\tau(u_0)$ does not exist and hence the cross cosine terms do not vanish when we take the limit. We now show that integrating $P_\tau(u)$ over a small non-zero interval $[u_0, u_0 + \alpha]$ and then taking the limit with respect to τ (followed by the limit with respect to α) does yield the density of Y.

From Lemmas (2.1) and (2.3), we see that for a given $a \in \mathcal{A}_{u_0}$, when u is varied over the interval $\mathcal{J}_\eta = [u_0 - \eta, u_0 + \eta]$, the inverse function $(S')^{-1}(u)$ is well defined with $(S')^{-1}(u) \in \mathcal{N}_a$, where $\mathcal{N}_a$ is some small neighborhood around a. For each $a \in \mathcal{A}_{u_0}$, define the inverse function $(S'_a)^{-1}(u) : \mathcal{J}_\eta \to \mathcal{N}_a$ as

$$
(S'_a)^{-1}(u) = x \text{ iff } u = S'(x) \text{ and } x \in \mathcal{N}_a. \quad\quad\quad\quad (2.23)
$$

Unfortunately, when we move from a fixed value u_0 to a variable u defined in the interval $\mathcal{J}_\eta$, the locations x_k and x_l which previously were fixed in (2.21) now also vary over the interval $\mathcal{J}_\eta$. This makes the notation somewhat cumbersome and unwieldy. Using the inverse functions defined in (2.23) and defining $a_k \equiv x_k(u_0)$ [and consequently

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$a_l = x_l(u_0)$], we define $x_k(u) \equiv \left(S'_{a_k}\right)^{-1}(u)$ [and therefore $x_l(u) = \left(S'_{a_l}\right)^{-1}(u)$]
for $u \in \mathcal{J}_\eta$. Finally, define the functions $p_{kl}(u)$ and $q_{kl}(u)$ over $\mathcal{J}_\eta$ as

$$p_{kl}(u) \quad \equiv \quad S\left(x_k(u)\right) - S\left(x_l(u)\right) - u\left(x_k(u) - x_l(u)\right), \text{ and} \qquad (2.24)$$

$$q_{kl}(u) \quad \equiv \quad \frac{1}{\left|S''\left(x_k(u)\right)\right|^{\frac{1}{2}} \left|S''\left(x_l(u)\right)\right|^{\frac{1}{2}}}. \qquad (2.25)$$

Observe that

$$p'_{kl}(u) \quad = \quad S'(x_k(u))x'_k(u) - S'(x_l(u))x'_l(u) - (x_k(u) - x_l(u)) - u\left(x'_k(u) - x'_l(u)\right)$$

$$= \quad x_l(u) - x_k(u) \qquad (2.26)$$

as $u = S'(x_k(u)) = S'(x_l(u))$. In particular, if $x_l(u_0) > x_k(u_0)$, then $x_l(u) > x_k(u)$
and vice versa. Hence, $p'_{kl}(u)$ never vanishes and is also of constant sign over $\mathcal{J}_\eta$.
Then, it follows that $p_{kl}(u)$ is *strictly monotonic* and specifically bijective on $\mathcal{J}_\eta$. We
will use this result in the subsequent steps.

Now, let $|\alpha| < \eta$. Since the additional error term $\epsilon_4(u_0, \tau)$ in (2.21) converges to
zero as $\tau \to 0$ and can also be *uniformly bounded* by a function of u_0 for small values
of τ, we have

$$\lim_{\tau \to 0} \int_{u_0}^{u_0+\alpha} \epsilon_4(u_0, \tau) du = 0. \qquad (2.27)$$

Then, we get

$$\lim_{\tau \to 0} \int_{u_0}^{u_0+\alpha} P_\tau(u) du = I_1 + I_2 \qquad (2.28)$$

where

$$I_1 \quad \equiv \quad \frac{1}{L} \sum_{k=1}^{N(u_0)} \int_{u_0}^{u_0+\alpha} \frac{1}{\left|S''\left(x_k(u)\right)\right|} du, \text{ and} \qquad (2.29)$$

$$I_2 \quad \equiv \quad \frac{1}{L} \sum_{k=1}^{N(u_0)} \sum_{l=1; l \neq k}^{N(u_0)} \lim_{\tau \to 0} I_3(k, l). \qquad (2.30)$$

Here, $I_3(k, l)$ is given by

$$I_3(k, l) \equiv \int_{u_0}^{u_0+\alpha} q_{kl}(u) \cos\left[\frac{p_{kl}(u)}{\tau} + \theta\left(x_k(u), x_l(u)\right)\right] du. \qquad (2.31)$$

When $|\alpha| < \eta$, the sign of $S''\left(x_k(u)\right)$ around $x_k(u_0)$ and the sign of $S''\left(x_l(u)\right)$
around $x_l(u_0)$ do not change over the interval $[u_0, u_0 + \alpha]$. Since $\theta(x_k(u), x_l(u))$ de-
pends on the sign of S'', θ is constant on $[u_0, u_0+\alpha]$ and equals $\theta_{kl} = \theta(x_k(u_0), x_l(u_0))$.

Now, expanding the cosine term in (2.31), we get

$$I_3(k,l) = \cos(\theta_{kl}) \int_{u_0}^{u_0+\alpha} q_{kl}(u) \cos\left(\frac{p_{kl}(u)}{\tau}\right) du$$

$$- \sin(\theta_{kl}) \int_{u_0}^{u_0+\alpha} q_{kl}(u) \sin\left(\frac{p_{kl}(u)}{\tau}\right) du. \qquad (2.32)$$

Since $p_{kl}(u)$ is bijective, we get via a standard change of variables:

$$I_3(k,l) = \cos(\theta_{kl}) I_4(k,l) - \sin(\theta_{kl}) I_5(k,l) \qquad (2.33)$$

where

$$I_4(k,l) = \int_{\beta_{kl}^{(1)}}^{\beta_{kl}^{(2)}} \cos\left(\frac{v}{\tau}\right) g_{kl}(v) dv, \text{ and} \qquad (2.34)$$

$$I_5(k,l) = \int_{\beta_{kl}^{(1)}}^{\beta_{kl}^{(2)}} \sin\left(\frac{v}{\tau}\right) g_{kl}(v) dv. \qquad (2.35)$$

Here, $\beta_{kl}^{(1)} = p_{kl}(u_0)$, $\beta_{kl}^{(2)} = p_{kl}(u_0 + \alpha)$ and $g_{kl}(v) = \frac{q_{kl}(p_{kl}^{-1}(v))}{p_{kl}'(p_{kl}^{-1}(v))}$.

Integrating $I_4(k,l)$ by parts, we get

$$I_4(k,l) = \tau \sin\left(\frac{\beta_{kl}^{(2)}}{\tau}\right) g_{kl}\left(\beta_{kl}^{(2)}\right) - \tau \sin\left(\frac{\beta_{kl}^{(1)}}{\tau}\right) g_{kl}\left(\beta_{kl}^{(1)}\right)$$

$$- \tau \int_{\beta_{kl}^{(1)}}^{\beta_{kl}^{(2)}} \sin\left(\frac{v}{\tau}\right) g_{kl}'(v) dv. \qquad (2.36)$$

Then,

$$|I_4(k,l)| \leq \tau \left(g_{kl}\left(\beta_{kl}^{(2)}\right) + g_{kl}\left(\beta_{kl}^{(1)}\right) + \int_{\beta_{kl}^{(1)}}^{\beta_{kl}^{(2)}} |g_{kl}'(v)| \, dv \right). \qquad (2.37)$$

It is worth mentioning that q_{kl} and hence g_{kl} are differentiable over their respective intervals as the sign of $S''(x_k(u))S''(x_l(u))$ does not change over the interval $[u_0, u_0 + \alpha]$. We then have $|I_4(k,l)| \leq \tau M$ where M is some constant independent of τ. Hence, $\lim_{\tau \to 0} I_4(k,l) = 0, \forall k,l$. By a similar argument, $\lim_{\tau \to 0} I_5(k,l) = 0, \forall k,l$. From (2.30) and (2.33), we get $I_2 = 0$. Since

$$\lim_{\alpha \to 0} \frac{1}{\alpha} I_1 = \frac{1}{L} \sum_{k=1}^{N(u_0)} \frac{1}{|S''(x_k)|} = P(u_0), \qquad (2.38)$$

the main result expressed in Theorem (2.5) follows. $\qquad \square$

Below, we show comparisons between our Fourier transform approach and the standard histogramming technique on some trigonometric and exponential functions sampled on a regular grid between $[-0.125, 0.125]$ at a grid spacing of $\frac{1}{2^{15}}$. For the sake of convenience, we normalized the functions such that its maximum gradient value is 1. Using the sampled values $\hat{S}$, we computed the Fast Fourier transform of $\exp\left(\frac{i\hat{S}}{\tau}\right)$ at $\tau = 0.00001$, took its magnitude squared and then normalized it to compute the gradient density. We also computed the discrete derivative of S at the grid locations and then determined its gradient density by histogramming using around 220 bins. The plots shown in Figure (1) provide anecdotal empirical evidence supporting the mathematical result stated in Theorem (2.5). Notice the near-perfect match between the gradient densities computed via standard histogramming and the gradient densities determined using our Fourier transform method.
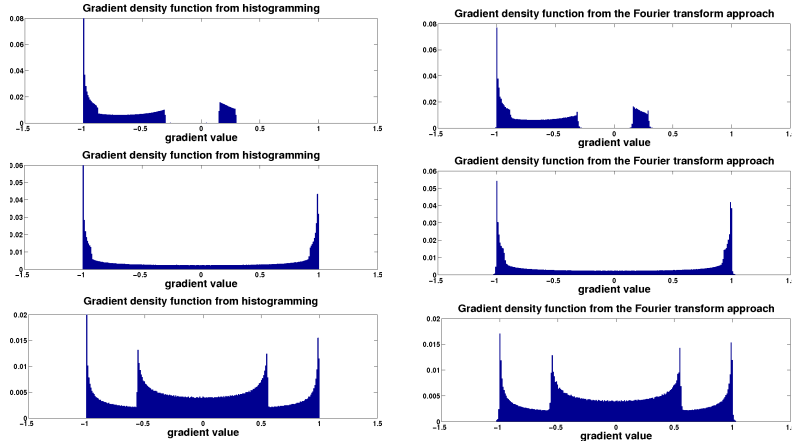

Figure 1: Comparison results. (i) Left: Gradient densities obtained from histogramming, (ii) Right : Gradient densities obtained from squared Fourier transform of the wave function

3. Discussion

Observe that the integrals

$$I_\tau(u_0) = \int_{u_0}^{u_0+\alpha} P_\tau(u)du, \quad I(u_0) = \int_{u_0}^{u_0+\alpha} P(u)du \tag{3.1}$$

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give the interval measures of the density functions P_τ and P respectively. Theorem (2.5) states that at small values of τ, both the interval measures are approximately equal, with the difference between them being $o(1)$. Recall that by definition, P_τ is the normalized power spectrum [see Bracewell (1999)] of the wave function $\phi(x) = \exp\left(\frac{iS(x)}{\tau}\right)$. Hence, we conclude that the power spectrum of $\phi(x)$ can potentially serve as a *density estimator* for the gradients of S at small values of τ. The experimental results shown above serve as a demonstration, anecdotally attesting to the verity of the result.

Our result is directly inspired by the three-way relationships between the classical momentum ∇S, the quantum momentum operator $-i\hbar\frac{\partial}{\partial x}$ and its spatial frequency spectrum. Since these relationships hold in higher dimensions as well, we are likewise interested in extending our density estimation result to higher dimensions. This is a fruitful avenue for future work.

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AppendixA. Proof of Lemmas

1. Proof of Finiteness Lemma

We prove the result by contradiction. Observe that $\mathcal{A}_u$ is a subset of the compact set Ω. If $\mathcal{A}_u$ is not finite, then by Theorem (2.37) in Rudin (1976), $\mathcal{A}_u$ has a limit point $x_0 \in \Omega$. Consider a sequence $\{x_n\}_{n=1}^{\infty}$, with each $x_n \in \mathcal{A}_u$, converging to x_0. Since $S'(x_n) = u, \forall n$, from the continuity of S' we get $S'(x_0) = u$ and hence $x_0 \in \mathcal{A}_u$. Then

$$\lim_{n \to \infty} \frac{S'(x_0) - S'(x_n)}{x_0 - x_n} = 0 = S''(x_0). \tag{A.1}$$

Based on the definitions given in (2.2), we have $x_0 \in \mathcal{B}$ and hence $u \in \mathcal{C}$ resulting in a contradiction. $\qquad\square$

2. Proof of Interval Lemma

Observe that $\mathcal{B}$ is closed because if x_0 is a limit point of $\mathcal{B}$, from the continuity of S'' we have $S''(x_0) = 0$ and hence $x_0 \in \mathcal{B}$. $\mathcal{B}$ is also compact as it is a closed subset of Ω. Since S' is continuous, $\mathcal{C} = S'(\mathcal{B}) \cup \{S'(b_1), S'(b_2)\}$ is also compact and hence $\mathbb{R} - \mathcal{C}$ is open. Then for $u \notin \mathcal{C}$, there exists an open neighborhood $\mathcal{N}_r(u)$ for some $r > 0$ around u such that $\mathcal{N}_r(u) \cap \mathcal{C} = \emptyset$. By defining $\eta = \frac{r}{2}$, the proof is complete. $\quad\square$

3. Proof of Density Lemma

Since the random variable X is assumed to have a uniform distribution on Ω, its density is given by $f_X(x) = \frac{1}{L}$ for every $x \in \Omega$. Recall that the random variable Y is obtained via a random variable transformation from X, using the function S'. Hence, its density function exists on $\mathbb{R} - \mathcal{C}$— where we have banished the image (under S') of the measure zero set of points where S'' vanishes—and is given by (2.3). The reader may refer to Billingsley (1995) for a detailed explanation. $\qquad\square$