On Numerical Estimation of Joint Probability Distribution from Lebesgue Integral Quadratures

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An important application of Lebesgue integral quadrature[1] is developed. Given two random processes, \( f(x) \) and \( g(x) \), two generalized eigenvalue problems can be formulated and solved. In addition to obtaining two Lebesgue quadratures (for \( f \) and \( g \)) from two eigenproblems, the projections of \( f \)- and \( g \)- eigenvectors on each other allow to build a joint distribution estimator, the most general form of which is a density–matrix correlation. Examples of the density–matrix correlation can be a value–correlation \( V_{[i],g[j]} \), similar to a regular correlation concept, and a new one, a probability–correlation \( P_{[i],g[j]} \). If Christoffel function average is used instead of regular average the approach can be extended to an estimation of joint probability of three and more random processes. The theory is implemented numerically; the software is available under the GPLv3 license.
I. INTRODUCTION

The Gaussian quadrature relatively a measure can be viewed as an optimal discrete interpolation of the measure; an application of the Gaussian quadrature to a function can be viewed as a Riemann integral sum. In [1] a new type of quadrature, producing the Lebesgue integral was introduced and applied to the problem of optimal discretization of a random process. In this paper a new application of the Lebesgue quadrature is developed. Assume one has two or more random processes \( f(x) \) and \( g(x) \). An application of the Lebesgue quadrature to each of them gives a set of (eigenvalue, eigenvector) pairs for \( f \) and \( g \). Projecting \( f \)– and \( g \)–eigenvectors on each other allows an estimator of joint \((f,g)\) distribution to be obtained:

\[
f(x)\text{ and } g(x)\text{ to have } n \text{ levels each (equal to their Lebesgue quadrature value–nodes } f[i] \text{ and } g[i]), \text{ the projections of eigenvectors define joint probability } (f = f[i]) \cap (g = g[j]), \text{ the most general form of which is a density–matrix correlation. The examples of the density–matrix correlation can be, introduced in [2], the value–correlation } V_{f[i],g[j]}, \text{ similar to a regular correlation concept, and a new one, a probability–correlation } P_{f[i],g[j]}. \text{ A problem of three–processes joint distribution can be approached and an estimation of joint probability of three and more random processes obtained if Christoffel function average is used instead of regular average.}

II. JOINT DISTRIBUTION ESTIMATION

In the work [1] a concept of the Lebesgue integral quadrature was introduced and optimal estimator of random process \( f(x) \) distribution was obtained by solving generalized eigenvalue problem

\[
\sum_{k=0}^{n-1} \langle Q_j \mid f \mid Q_k \rangle \alpha_{f[i]}^k = \lambda_f^i \sum_{k=0}^{n-1} \langle Q_j \mid Q_k \rangle \alpha_{f[i]}^k \tag{1}
\]

\[
\psi_f^i(x) = \sum_{k=0}^{n-1} \alpha_{f[i]}^k Q_k(x) \tag{2}
\]

The value–nodes and weights of Lebesgue integral quadrature:

\[
f[i] = \lambda_f^i \tag{3}
\]

\[
w_f^i = \langle \psi_f^i \rangle^2 \tag{4}
\]

\(^1\) An important feature of the approach is its applicability to the signals with spikes, fat tails, infinite \( \langle f^2 \rangle, \langle fg \rangle, \text{ or } \langle g^2 \rangle, \text{ etc., because eigenvalue problem } [1] \text{ is stable and well defined for such } f(x) \text{ and } g(x). \text{ The approach cannot be applied to the processes with infinite } \langle f \rangle \text{ or } \langle g \rangle \text{ as this leads to infinite } \langle Q_j \mid f \mid Q_k \rangle \text{ or } \langle Q_j \mid g \mid Q_k \rangle.\]
is optimal \( n \)-point discrete distribution, producing Lebesgue integral \( df \) relatively the measure \( d\mu \) (if \( f(x) = x \) then \( f^{[i]} \) and \( w_f^{[i]} \) are the nodes and the weights of Gaussian quadrature, optimal Riemann integral sum). The weights \( w_f^{[i]} \) of the Lebesgue integral quadrature is the measure of \( f = f^{[i]} \) sets. Now assume one has two random processes \( f(x) \) and \( g(x) \) and want to obtain not only \( f \)– and \( g \)– distributions (from the Lebesgue integral quadrature), but also to obtain the measure of \( (f = f^{[i]} \cap g = g^{[j]} \) sets, a joint distribution of \( (f, g) \).

As we emphasized in \[1\] any quadrature is defined by \( n \) (eigenvalue, eigenvector) pairs of \( f \) problem: \( (\lambda_f^{[i]}, \psi_f^{[i]}) \). One can solve \( \int f(x) \, d\mu \) with \( g(x) \) (instead of \( f(x) \)) and obtain one more set of \( n \) pairs \( (\lambda_g^{[i]}, \psi_g^{[i]}) \). Because right hand side of \( \int f(x) \, d\mu \) is the same for \( f(x) \) and \( g(x) \), the eigenvectors for \( f \) and \( g \) can be projected to each other as: \( \langle \psi_f^{[i]} \mid \psi_g^{[j]} \rangle = \sum_{m,m'} \alpha_{m,m'}^{[i]} \langle Q_m \mid Q_{m'} \rangle \alpha_{m'}^{[j]} \).

Consider total measure \( \int d\mu \), taking into account \( \int d\mu = 1 = \sum_{i,j=0}^{n-1} \langle \psi_f^{[i]} \mid \psi_g^{[j]} \rangle \langle \psi_f^{[i]} \mid \psi_g^{[j]} \rangle \) obtain:

\[
\begin{align*}
\int d\mu = 1 &= \sum_{i,j=0}^{n-1} \langle \psi_f^{[i]} \mid \psi_g^{[j]} \rangle \\
V_{f[i],g[j]} &= \langle \psi_f^{[i]} \mid \psi_g^{[j]} \rangle \\
\sum_{i,j=0}^{n-1} V_{f[i],g[j]} &= 1 \quad (5) \\
\sum_{j=0}^{n-1} V_{f[i],g[j]} &= w_f^{[i]} \quad (6) \\
\sum_{i=0}^{n-1} V_{f[i],g[j]} &= w_g^{[j]} \quad (7)
\end{align*}
\]

When \( f = g \) then the matrix \( V_{f[i],g[j]} \) is diagonal, the diagonal elements are equal to the Lebesgue integral quadrature weights \( (4) \). In general case \( (6) \) matrix elements can be considered as Lebesgue measure of \( (f = f^{[i]} \cap g = g^{[j]} \) sets, this matrix is related to joint distribution matrix of \( (f, g) \) relatively the measure \( d\mu \). However, in contrast with the Lebesgue integral quadrature weights \( w_f^{[i]} \) and \( w_g^{[i]} \), the \( V_{f[i],g[j]} \) elements are not always positive, but are still useful for \( (f, g) \) joint probability estimation; obtained joint distribution matrix is correct “on average”: \( (8) \) and \( (9) \).

One more matrix \( P_{ij} \) can be introduced:

\[
\begin{align*}
P_{f[i],g[j]} &= \langle \psi_f^{[i]} \mid \psi_g^{[j]} \rangle^2 \\
\sum_{i,j=0}^{n-1} P_{f[i],g[j]} &= n \quad (10)
\end{align*}
\]
The $P_{f[i],g[j]}$ matrix is always positive but is normalized to eigenvalues number $n$, not to the total measure $\langle 1 \rangle$ as $V_{f[i],g[j]}$ is.

The $V_{f[i],g[j]}$ and $P_{f[i],g[j]}$ joint distributions matrices are a generalization of value–correlation and probability–correlation concepts introduced in Ref. \[2\] for $n = 2$ case. For $n = 2$ the $(P_{f[i],g[j]} + P_{f[i],g[j]} - P_{f[i],g[j]} - P_{f[i],g[j]})/2$ is exactly the $\tilde{p}(f, g)$ of Ref. \[2\] Appendix C, $P_{f[i],g[j]}$ has the meaning of probability of probability for $f = f[i]$ and $g = g[j]$; $V_{f[i],g[j]}$ has the meaning of probability (measure) for $f = f[i]$ and $g = g[j]$ and normalizing $\langle 7 \rangle$, it is different from $L^4$ covariation of Ref. \[2\] Appendix B, only in basis choice. These two correlation concepts are a special case of the density matrix correlation concept.

## A. Density Matrix Correlation

Obtained (6) and (10) joint probability estimators can be generalized as

$$P_{f[i],g[j]} = \langle \psi_f^{[i]} \rvert \psi_g^{[j]} \rangle \langle \psi_f^{[i]} \rvert \rvert \psi_g^{[j]} \rangle$$

\quad (12)

$$\sum_{i,j=0}^{n-1} P_{f[i],g[j]} = \text{Spur} \bigr\| \rho \bigr\|$$

\quad (13)

where $\bigr\| \rho \bigr\|$ is a “density matrix” operator, $f$ and $g$ averages are now Spur $\bigr\| \rho \rvert f \bigr\|$ and Spur $\bigr\| \rho \rvert g \bigr\|$, with normalizing (13). The $\bigr\| \rho \bigr\| = \langle 1 \rangle \langle 1 \rangle$ gives regular average and value–correlation (6), the $\bigr\| \rho \bigr\| = \langle 1 \rangle$ gives the number of eigenvalues as average and probability–correlation (10). For a given polynomial $P(x)$ of $2n - 2$ degree, density matrix $\bigr\| \rho \bigr\|$ operator can be constructed according to Ref.\[1\] Appendix A algorithm, where, for a given polynomial, an operator $\bigr\| \rho \bigr\|$ has been obtained, such that:

$$\rho(x, y) = \sum_{i=0}^{n-1} \psi^{[i]}(x) \lambda^{[i]} \psi^{[i]}(y)$$

\quad (14)

$$P(x) = \rho(x, x)$$

\quad (15)

with $\lambda^{[i]}; \psi^{[i]}(x)$ the eigenvalues and the eigenvectors of $\bigr\| \rho \bigr\|$. In a general case the sign of matrix elements, same as for (9), is not always positive what allows only “on average” interpretation. One may consider a different type of estimation:

$$P_{f[i],g[j]} = \langle \psi_f^{[i]} \rvert \rvert \psi_g^{[j]} \rangle^2$$

\quad (16)

where the density matrix is used in both terms in (12). For $\bigr\| \rho \bigr\| = \langle 1 \rangle \langle 1 \rangle$ the weight of $(f = f[i]) \cap (g = g[j])$ is equal to the product of Lebesgue quadrature weights for $f$ and $g$.
quadratures:

\[
P_{f^i|g^j} = \left< \psi^i_f \right| \left< \psi^j_g \right>^2 = \left< \psi^i_f \right| \left< \psi^j_g \right>^2
\]

\[
\sum_{i,j=0}^{n-1} P_{f^i|g^j} = \langle 1 \rangle^2
\]

with (18) normalizing. The (17) is “uncorrelated” answer, where the probability of joint \((f, g)\) distribution is equal to the product of individual distributions. Such “uncorrelated” answers always arise for pure states, the states with the density matrix in \(\|\rho\| = |\psi\rangle \langle \psi|\) form. In general case, such as (14), obtained joint distribution does not factorize.

III. NUMERICAL ESTIMATION

Numerical estimation is not much different from the Lebesgue integral quadrature calculation in Ref. [1]. With a good choice for \(Q_k(x)\) basis the problem can be efficiently solved for a very large \(n\). Once the \(\langle Q_m \rangle, \langle fQ_m \rangle, \) and \(\langle gQ_m \rangle\) moments are obtained for \(m = 0 \ldots 2n - 1\), the matrices \(\langle Q_j | Q_k \rangle, \langle Q_j | f | Q_k \rangle, \) and \(\langle Q_j | g | Q_k \rangle, j, k = 0 \ldots n - 1\), can be calculated using basis functions multiplication operator, and eigenvalue problem (1) can be solved using e.g. generalized eigenvalue subroutines from Lapack [7]. In practical application it is better to solve generalized eigenvalue problem for \(f(x)\) first, obtain \(\psi_f^i(x)\). Then generalized eigenvalue problem for \(g(x)\) can be written in \(\psi_f^i(x)\) basis \(\sum_{k=0}^{n-1} \left< \psi_f^j \right| g \left| \psi_f^k \right> \alpha_k^{q^i} = \lambda^i_g \sum_{k=0}^{n-1} \left< \psi_f^j \right| \psi_f^k \right> \alpha_k^{q^i},\) that has unit right hand side matrix: \(\left< \psi_f^i \right| \psi_f^j \right> = \delta_{jk}\), and can be solved using regular eigenvalue subroutines, what both optimizes the code and increases numerical stability of calculations. Provided java–implementation [8], file code_polynomials_quadratures.zip the methods getValueCorrelation, getProbabilityCorrelation, and getDensityMatrixCorrelation of com/polytechnik/utils/LebesgueQuadratureJointDistribution.java a class, constructed from two Lebesgue quadratures as input, calculate correlation matrices. Octave file LebesgueQuadratures_call_java_example.m is usage demonstration of this java implementation application to sampled data. Given \(l = 1 \ldots M\) sample

\[
x^{(l)} \rightarrow f^{(l)}, g^{(l)}\quad \text{weight } \omega^{(l)}
\]
the matrices

\[ \langle Q_j | Q_k \rangle = \sum_{l=1}^{M} Q_j(x^{(l)})Q_k(x^{(l)})\omega^{(l)} \] (20)

\[ \langle Q_j | f | Q_k \rangle = \sum_{l=1}^{M} Q_j(x^{(l)})Q_k(x^{(l)})f^{(l)}\omega^{(l)} \] (21)

\[ \langle Q_j | g | Q_k \rangle = \sum_{l=1}^{M} Q_j(x^{(l)})Q_k(x^{(l)})g^{(l)}\omega^{(l)} \] (22)

are calculated from sampled data. For implementation demonstration a subset of java library functionality is also implemented in native octave language in `com/polytechnik/utils/LebesgueQuadraturesJointDistribution.m`, see usage demonstration in `LebesgueQuadratures.m`. The results of java and octave implementations are identical.

IV. CHRISTOFFEL FUNCTION AVERAGE AND JOINT DISTRIBUTION OF THREE RANDOM PROCESSES.

Obtained joint probability estimator (12) uses projections of \( f \)– and \( g \)– eigenvectors on each other. This approach, besides “negative probability” interpretation difficulty cannot directly estimate a joint distribution of three or more processes.

\[ (x_0, x_1, \ldots, x_k, \ldots, x_{n-1})^{(l)} \rightarrow f^{(l)}, g^{(l)}, e^{(l)}, \ldots \] weight \( \omega^{(l)} \) (23)

When eigenvalue/eigenvectors pairs \((\lambda_s^{[i]}, \psi_s^{[i]})\) are obtained for each \( s = f, g, e, \ldots \):

\[ |s|\psi_s^{[i]} = \lambda_s^{[i]} |\psi_s^{[i]} \rangle \] (24)

a three–function projection cannot be directly obtained for say \( |\psi_f^{[i]} \rangle \), \( |\psi_g^{[j]} \rangle \), and \( |\psi_e^{[k]} \rangle \).

However, a three–function joint distribution estimator can be obtained with a Christoffel function average; the concept was originally introduced in [9] (as Eq. (20) therein) and recently was applied in [10] to the Low Rank Representation (LRR) problem of a matrix.

Consider a \( x = y \) localized state \( \psi_y(x) \):

\[ \psi_y(x) = \frac{\sum_{i=0}^{n-1} \psi_y^{[i]}(y) \psi_y^{[i]}(x)}{\sqrt{\sum_{i=0}^{n-1} [\psi_y^{[i]}(y)]^2}} = \frac{\sum_{j,k=0}^{n-1} y_j G_{jk}^{-1} x_k}{\sqrt{\sum_{j,k=0}^{n-1} y_j G_{jk}^{-1} y_k} } \] (25)

\[ 2 \text{ Here we also consider } x \text{–space to be a vector space of arbitrary origin; the consideration of above corresponds to these components being polynomials of some real variable: } x_k = Q_k(x) \]
Here $G_{jk} = \langle x_j \mid x_k \rangle$ is Gram matrix; in one-dimensional case it is $G_{jk} = \langle Q_j \mid Q_k \rangle$ in right hand side of (1). Averaging with $\psi_y^2$ gives Radon–Nikodym approximation at $y$.

The Christoffel function average of a $x$–dependent function $\phi(x)$ is defined as:

- Calculate the $\langle \psi_y \mid \phi \mid \psi_y \rangle$ according to the measure (23), obtain $y$–dependent function. This is just regular $\psi$ average we used here and in all our previous works. This average of $\phi(x)$ with $\psi_y^2(x)$ is it’s Radon–Nikodym approximation at $y$.

- Average obtained $y$–dependent function over all $y \in x(l)$, $l = 1 \ldots M$ with the weights $\omega(l)$:

$$
\langle \phi \rangle_{\text{Christoffel}} = \sum_{l=1}^{M} \omega(l) \langle \psi_y(l) \mid \phi \mid \psi_y(l) \rangle = \sum_{l=1}^{M} \omega(l) \sum_{l'=1}^{M} \omega(l') \phi(x(l')) \psi_y^2(l)(x(l'))
$$

While regular averaging

$$
\langle \phi \rangle = \sum_{l=1}^{M} \omega(l) \phi(y(l))
$$

uses the value $\phi(y(l))$ to average, the Christoffel function average uses it’s Radon–Nikodym approximation $\langle \psi_y(l) \mid \phi \mid \psi_y(l) \rangle$ instead. For a large enough $n$ the result is similar. Since Radon–Nikodym approximation preserves the normalizing and sign we also have: $\langle 1 \rangle_{\text{Christoffel}} = \langle 1 \rangle$.

The key Christoffel average feature is that we can represent it in any basis: because the $\psi_y(x)$ is a regular wavefunction, it can be expanded in any full basis, for example (24). For $\psi_s^{[i]}(x)$, $s = f, g, e, \ldots$, taking into account basis functions orthogonality, obtain:

$$
\psi_y(x) = \sum_{i=0}^{n-1} \langle \psi_s^{[i]} \mid \psi_y \rangle \psi_s^{[i]}(x)
$$

$$
\langle s \rangle_{\text{Christoffel}} = \sum_{l=1}^{M} \omega(l) \langle \psi_y(l) \mid s \mid \psi_y(l) \rangle = \sum_{l=1}^{M} \omega(l) \sum_{i=0}^{n-1} \lambda_s^{[i]} \langle \psi_y(l) \mid \psi_s^{[i]} \rangle^2
$$

$$
1 = \sum_{i=0}^{n-1} \langle \psi_y(l) \mid \psi_s^{[i]} \rangle^2
$$

The Christoffel function average $\langle s \rangle_{\text{Christoffel}}$ is an average of $l = 1 \ldots M$ observations, where each one is a probability distribution of $n$ outcomes $\lambda_s^{[i]}$ (the (24) eigenvalues) with the weights $\omega(l) \langle \psi_y(l) \mid \psi_s^{[i]} \rangle^2$; the regular average $\langle s \rangle$ is a superposition of $l = 1 \ldots M$ observations $s^{(l)}$ with the weights $\omega(l)$. 
A remarkable feature of (29) is that it has the same representation for any \( s = f, g, e, \ldots \). The most straightforward approach to obtain joint distribution is, for a given \( l \), to consider the components to be independent (this is reasonable because for a large \( n \) only a single coefficient \( \langle \psi_y | \psi^{[k]} \rangle^2 \) is typically large) hence one can consider the joint probability at \( y^{(l)} \) to be a product \( \langle \psi_y | \psi^{[i]} \rangle^2 \langle \psi_y | \psi^{[j]} \rangle^2 \langle \psi_y | \psi^{[k]} \rangle^2 \). The joint probability is then:

\[
P_{f^{[i]}, g^{[j]}, e^{[k]}} = P \left( f = f^{[i]} \cap g = g^{[j]} \cap e = e^{[k]} \right) = \sum_{l=1}^{M} \omega^{(l)} \langle \psi_y | \psi^{[i]} \rangle^2 \langle \psi_y | \psi^{[j]} \rangle^2 \langle \psi_y | \psi^{[k]} \rangle^2
\]

(31)

This joint probability estimator is always positive, has proper normalizing, and can be used to estimate joint distribution of three or more random processes. In one-dimensional case it gives outcome weights equal to Christoffel function diagonal elements in the basis \( |\psi^{[i]}_j\rangle \). For \( f = g = e \) it produces properly diagonal joint distribution matrix \( P \left( f = f^{[i]} \cap g = g^{[j]} \cap e = e^{[k]} \right) \approx 0 \) for \( i \neq j \neq k \) only for a large enough \( n \), this is a limitation of this estimator.

We see (31) as an extremely promising path to vector-valued class label machine learning. The Christoffel function joint probability estimator combines the spectral approach (24) success for scalar class label of Ref. [10] with a vector class label \( \mathbf{f} = (f, g, e, \ldots) \).

V. CONCLUSION

Obtained in Ref. [1] a new class of quadratures, the Lebesgue quadrature, can be applied not only to optimal discretization of a random process by a \( n \)-point discrete Lebesgue measure, but also to a numerical estimation of joint distribution of \((f(x), g(x))\). The most general form is density matrix correlation. Introduced in Ref. [2] Appendix B, value–correlation [6] and probability–correlation [10] are special cases of density matrix correlation. If Christoffel function average is used instead of regular average the approach can be further extended (31) to three and more random processes. The software is available under the GPLv3 license.

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3 One can also try to consider the “two–particle” probability distribution like [10] with chain rule and decoupling.
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