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Efficient integration over the unitary group with applications

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Abstract: This paper describes efficient methods for integration polynomial functions on elements of the unitary group with respect to the Haar measure. Some methods for special cases are shown. Finally examples of applications are described.

Keywords: integration, unitary matrices

1. Introduction

The integrals of polynomial functions over the unitary group are important in many areas of science. Applications of such integration can be found in mathematical physics, random matrix theory, quantum information processing and algebraic combinatorics. The first mentions of the problem of integration of elements of unitary matrices can be found in literature in the context of nuclear physics [1].

There exists a package that performs integration of polynomial functions over the unitary group with respect to the Haar measure [2], however in case of polynomials of large degree, consisting of complex monomials, the computations are very time-consuming. In this paper we describe more efficient methods for calculating such integrals.

This paper is organised as follows. In Section 2 we recall Collins-Śniady formula [3] for calculating monomial integrals. The main contribution of this paper is provided in Section 3, where we described a practical algorithms for the calculation. We also provide a number of special cases which can be used to improve the calculation efficiency for some classes of monomial functions. Finally, in Section 4 we present some applications.

2. Mathematical background

In this section we introduce some basic definitions that we use in this paper. We form a definition of integral that can be computed with use of presented methods. Finally we introduce Collins-Śniady formula.

2.1. Basic definitions

We denote by $\lambda \vdash n$ a partition of n, i.e. a non-increasing sequence of positive integers $\lambda = (\lambda_1, \ldots, \lambda_k)$ such that $\sum_{i=1}^{k} \lambda_i = n$. A length of partition λ is denoted by $l(\lambda)$ and it is equal to the number of elements in sequence. Each permutation $\sigma \in S_n$ has unique representation as a sum of disjoint cycles. A non-increasing sequence of lengths of cycles of permutation forms a partition of n. This partition is called cycle type $\mathrm{ct}\sigma$ of permutation σ. An ordered concatenation of partitions λ_1, λ_2, which result is a partition λ is denoted as $\lambda = \lambda_1 \sqcup \lambda_2$. In this paper we denote cardinality of a set A as $|A|$ and we also use a Kronecker delta symbol $\delta_{i,j} = \begin{cases} 1 i = j, \\ 0 i \neq j. \end{cases}$.

2.2. Polynomial integrals

Consider set $\mathcal{M}_d$ of all square matrices of size d. Matrices $U \in \mathcal{M}_d$ such that $U^{-1} = U^\dagger$, where $U^\dagger$ is a hermitian conjugate of U, are called unitary matrices and forms a group $\mathrm{U}(d)$. There exists only one normalized measure which is right and left invariant under the group operation and it is called the Haar measure here denoted as dU [3]. In this paper we discuss integrals with respect to this special measure.

Because of the linearity of integral, the integral of polynomial function on the unitary group with respect to the Haar measure can be decomposed as:

$$\int\limits_{\mathrm{U}(d)} p(U)dU = \sum_{I,I',J,J'} c_{I,I',J,J'} \int\limits_{\mathrm{U}(d)} U_{i_1,j_1} \ldots U_{i_{n_k},j_{n_k}} \overline{U_{i_1,j_1} \ldots U_{i_{n'_k},j_{n'_k}}} dU, \tag{1}$$

where lists of indices in integrated monomials are denoted as multiindices $I = (i_1, \ldots, i_n), I' = (i'_1, \ldots, i'_n), J = (j_1, \ldots, j_{n'}), J' = (j'_1, \ldots, j'_{n'})$. For this reasoning in this paper we consider only the integrals of monomial functions:

$$\int_{\mathrm{U}(d)} U_{i_1,j_1} \ldots U_{i_n,j_n} \overline{U_{i'_1,j'_1} \ldots U_{i'_{n'},j'_{n'}}} dU. \tag{2}$$

Such monomial integrals are known as moments of $\mathrm{U}(d)$.

2.3. Collins-Śniady formula

When lengths of multiindices I and J are equal we use following formula [3]:

$$\int_{\mathrm{U}(d)} U_{i_1,j_1} \dots U_{i_n,j_n} \overline{U_{i'_1,j'_1} \dots U_{i'_n,j'_n}} dU = \sum_{\sigma,\tau \in S_n} \delta_{i_1,i'_{\sigma(1)}} \dots \delta_{i_n,i'_{\sigma(n)}} \delta_{j_1,j'_{\tau(1)}} \dots \delta_{j_n,j'_{\tau(n)}} \mathcal{W}g(\tau\sigma^{-1}, n, d). \tag{3}$$

The formula is valid in the case when multiindices has the same length. In the opposite case the integral is equal to 0. Function $\mathcal{W}g$ used in formula (3) is called *Weingarten* function and is defined as follows:

$$\mathcal{W}g(\sigma, n, d) = \frac{1}{(n!)^2} \sum_{\substack{\lambda \vdash n \\ l(\lambda) \leq d}} \frac{\chi^\lambda(e)^2}{s_{\lambda,d}(1)} \chi^\lambda(ct\sigma). \tag{4}$$

The function is named after Don Weingarten, a mathematician who considered the asymptotic behavior of the integrals of type (2) [4]. In (4) $s_{\lambda,d}(1)$ is the Schur polynomial s_λ at the point $(\underbrace{1,\dots,1}_{d})$ and χ^λ is an irreducible character of the symmetric group S_n indexed by partition λ. The Schur polynomial evaluated at $(\underbrace{1,\dots,1}_{d})$ is the dimension of irreducible representation of $\mathrm{U}(d)$ corresponding to the partition λ. In this special case, its value is equal to [5]:

$$s_{\lambda,d}(1) = s_\lambda(\underbrace{1,\dots,1}_{d}) = \prod_{1 \leq i < j \leq d} \frac{\lambda_i - \lambda_j + j - i}{j - i}. \tag{5}$$

The irreducible character of S_n indexed by partition λ, $\chi^\lambda(\sigma)$ is defined for $\sigma \in S_n$. The value of $\chi^\lambda(\sigma)$ depends on a conjugacy class of a permutation σ. Each conjugacy class contains all permutations that have the same cycle type. It is common to define χ^λ for partitions, thus $\chi^\lambda(\sigma) = \chi^\lambda(\mu)$ when μ is cycle type of σ. When identity permutation is considered the cycle type is given by a trivial partition, $e = (\underbrace{1,\dots,1}_{n})$ and the value of the irreducible character is equal to dimension of the irreducible representation of S_n indexed by λ. In this case it is given by the formula [5]:

$$\chi^\lambda(e) = \frac{|\lambda|!}{\prod_{i,j} h^\lambda_{i,j}}, \tag{6}$$

where $|\lambda| = \lambda_1 + \lambda_2 + \cdots \lambda_{l(\lambda)}$ and $h^{\lambda}_{i,j}$ is the hook length of the cell (i, j) in a Ferrers diagram corresponding to partition λ. In other cases when non-trivial permutation(partition) is considered the character of symmetric group, $\chi^{\lambda}(\sigma) = \chi^{\lambda}(\mu)$ can be evaluated using Murnaghan-Nakayama rule. An efficient algorithm implementing Murnaghan-Nakayama rule can be found in [6].

3. Efficient computation

In this section we provide an efficient algorithm for calculating integrals of the type (2). We also present a number of special cases of integrals. In this cases a value of an integral can be calculated with use of less time-consuming methods.

3.1. General computation formula

Since Weingarden function depends on cycle type of permutation, rather than on a permutation itself $\mathcal{W}g$ can be defined as a function of integer partition:

$$\mathcal{W}g(\sigma, d, n) = \mathcal{W}g(\mu, d, n), \tag{7}$$

where $\mu = \mathrm{ct}\sigma$. It is reasonable to introduce function that represents number of permutations with certain cycle type that do not vanish in summation in formula (3):

$$N(\lambda) = \sum_{\substack{\sigma, \tau \in S_n \\ ct(\tau\sigma^{-1}) = \lambda}} \delta_{i_1,i'_{\sigma(1)}} \ldots \delta_{i_n,i'_{\sigma(n)}} \delta_{j_1,j'_{\tau(1)}} \ldots \delta_{j_n,j'_{\tau(n)}}. \tag{8}$$

In other words $N(\lambda)$ is size of equivalence class of λ in equivalence relation of $\mathcal{W}g(\lambda')$ for $\lambda' \vdash n$. In practical realisation values of $N(\lambda)$ are computed simultaneously for all partitions $\lambda \vdash n$ by computing factors $\delta_{\sigma\tau}$ for all products $\tau\sigma^{-1}$ and incrementing appropriate $N(\lambda)$. With such definition formula (3) can be restated:

$$\int U_{i_1,j_1} \ldots U_{i_n,j_n} \overline{U_{i'_1,j'_1} \ldots U_{i'_n,j'_n}} \mathrm{d}U = \sum_{\lambda \vdash n} N(\lambda) \mathcal{W}g(\lambda, n, d). \tag{9}$$

The aim of presenting this form is to show, that number of invoking function $\mathcal{W}g$ can be reduced to $O(B_n)$ instead of $O(n!^2)$, where B_n is the Bell number [7].

Now let us simplify notation of discussed formula by introducing sets of permutations that do not vanish in summation (3) $S_{I,I'} = \{\sigma \in S_n : \delta_{i_1,i'_{\sigma(1)}} \ldots \delta_{i_n,i'_{\sigma(n)}} = 1\}$ and $S_{J,J'} = \{\tau \in S_n : \delta_{j_1,j'_{\tau(1)}} \ldots \delta_{j_n,j'_{\tau(n)}} = 1\}$ that represents permutations which factors in formula (3) are non-zero. Now, function N defined in equation (8) is equal to

$$N(\lambda) = |\{(\sigma, \tau) \in S_{I,I'} \times S_{J,J'} : ct(\tau\sigma^{-1}) = \lambda\}|. \tag{10}$$

It is obvious that $\sigma \in S_{I,I'} \iff \sigma(I) = I'$ and $\tau \in S_{J,J'} \iff \tau(J) = J'$.

In formula (3) we compute all possible products $\tau\sigma^{-1}$ such that $\sigma \in S_{I,I'}$ and $\tau \in S_{J,J'}$. List of all such products may contain equal elements. Thus it is possible that distinct pairs $(\sigma, \tau), (\sigma', \tau') \in S_{I,I'} \times S_{J,J'}$ have equal product $\tau\sigma^{-1} = \tau'\sigma'^{-1}$. Since only number of particular permutations is needed computing the same permutation more than one time is inefficient. In this section we study possibility to count number of distinct pairs $(\sigma, \tau) \in S_{I,I'} \times S_{J,J'}$ with equal product $\tau\sigma^{-1}$.

Fact 1 If $\sigma^{-1}(J') = \sigma'^{-1}(J')$ and $\sigma \neq \sigma'$ then for every $\tau \in S_{J,J'}$ there is $\tau \neq \tau' \in S_{J,J'}$ that $\tau\sigma^{-1} = \tau'\sigma'^{-1}$.

Proof: When $\sigma^{-1}(J') = \sigma'^{-1}(J')$ then there is permutation ϕ that $\sigma^{-1} = \phi\sigma'^{-1}$. Then for each permutation $\tau \in S_{J,J'}$ permutation $\tau\phi^{-1} \in S_{J,J'}$. When $\tau' = \tau\phi^{-1}$ then $\tau'\sigma'^{-1} = \tau\phi^{-1}\phi\sigma^{-1} = \tau\sigma^{-1}$. □

Fact 1 implies that all permutations included in sum (10) can be obtained from some reduced set $S'_{I,I'}$ instead of $S_{I,I'}$. Set $S'_{I,I'}$ can be defined as set of all permutations from $S_{I,I'}$ which inversions have unique image of J'.

Fact 2 Number of different permutations in $S_{I,I'}$ such that theirs inversions have equal image on J' is equal to

$$c = |\{\sigma' \in S_{I,I'} : \sigma'(J') = \sigma(J')\}| = \prod_{i \in I'} \prod_{j \in J'} \Big(\sum_{1 \leq k \leq d} \delta_{I'(k),i}\delta_{J'(k),j} \Big)!.$$

Proof: Let us define a set $S^e_{I',J'}$ of all permutation that do not change multiindices I' and J': $S^e_{I',J'} = \{\sigma \in S_d : \sigma(I') = I' \wedge \sigma(J') = J'\}$. Each permutation in $S^e_{I',J'}$ permutes positions of I' and J' where indices are equal. Thus it can be decomposed as product of permutations of positions with equal elements. Let us divide all positions into sets $K_{i,j} = \{k : I'(k) = i \wedge J'(k) = j\}$ of positions with equal element in I' and J'. Then set $S^e_{I',J'}$ is a set of products of disjoint permutations of positions from all sets $K_{i,j}$ independently, thus $|S^e_{I',J'}| = \prod_{i \in I'} \prod_{j \in J'} |K_{i,j}|!$.

For any permutations $\sigma \in S_{I,I'}$ and $\phi \in S^e_{I'J'}$ permutation $\phi\sigma^{-1}$ has the same image of J' as σ^{-1} and there exists some permutation $\sigma' \in S_{I',J'}$ that $\sigma'^{-1} = \phi\sigma^{-1}$. Thus there are $|S^e_{I'J'}|$ permutations in $S_{I,I'}$ which inversions have the same image of J' that σ^{-1}. □

According to fact 2 using set $S'_{I,I'}$ that contains all permutations from $S_{I,I'}$ with unique image on J' it is possible to reduce number of computed permutations exactly c times.

$$N(\lambda) = c|\{(\sigma, \tau) \in S'_{I,I'} \times S_{J,J'} : ct(\tau\sigma^{-1}) = \lambda\}| \tag{11}$$

Introduced reduction of computed products of permutations is optimal. In set $\{(\sigma, \tau) \in S'_{I,I'} \times S_{J,J'}\}$ there are no two different pairs $(\sigma, \tau), (\sigma', \tau') \in S'_{I,I'} \times S_{J,J'}$ with equal product $\tau\sigma^{-1} = \tau'\sigma'^{-1}$.

Now during computation when sets $S'_{I,I'}$ and $S_{J,J'}$ are obtained it is possible to compute products of permutations from S on J' and form set $S'_{I,I'}$ with all permutations with unique product of J'. Now set $S'_{I,I'}$ can be used in further computation instead of set $S_{I,I'}$ and final result must be multiplied by c. Values of $N(\lambda)$ are obtained efficiently by getting all possible pairs $(\sigma, \tau) \in S'_{I,I'}, S_{J,J'}$ and incrementing value of $N(\lambda)$ such that $\mathrm{ct}(\tau\sigma^{-1}) = \lambda$ by c.

3.2. Special case 1: elements from one row

When all elements in polynomial function that is being integrated are in the same row (or column) there is much simpler way to compute integral. The distribution of random vector of squares of absolute values of row or a column of unitary matrix distributed with Haar measure is uniform on a standard d-simplex [8].

$$\int_{U(d)} \prod_{j=1}^{d} |U_{i_0,j}|^{2p_j} dU = \Gamma(d) \frac{\Gamma(p_1+1) \times \ldots \times \Gamma(p_d+1)}{\Gamma(p_1+\ldots+p_d+d)} \tag{12}$$

3.3. Special case 2: diagonal matrices

A special case of block diagonal matrix is a diagonal matrix. To use features of integrals of monomials containing elements from diagonal, we will use a fact;

Fact 3 For every integral of monomial and every permutations $\sigma, \tau \in S_d$ an equation occurs:

$$\int_{U(d)} U_{\sigma(i_1),\tau(j_1)} \ldots U_{\sigma(i_n),\tau(j_n)} \overline{U_{\sigma(i'_1),\tau(j'_1)} \ldots U_{\sigma(i'_n),\tau(j'_n)}} \mathrm{d}U = \tag{13}$$

$$\int_{U(d)} U_{i_1,j_1} \ldots U_{i_n,j_n} \overline{U_{i'_1,j'_1} \ldots U_{i'_n,j'_n}} \mathrm{d}U.$$

Proof: Such permutations are equal to permutations of rows and cols in matrix, what is invariant in integration over group.

For diagonal matrices all lists of indices are equal: $I = I' = J = J'$. According to definition of set $T = \{\tau \in S_d : \sigma(J) = J'\}$ if $J = J'$ then T is subgroup of S_d, and if J consists of indices $(1, \ldots, k)$ and index i occurs in J exactly l_i times, $i = 1, \ldots, k$, then T is a product of groups: $T = S_{l_1} S_{l_2} \ldots S_{l_k}$, where S_{l_i} is a group of all permutations in positions of index i for $i = 1, \ldots, k$.

To get number of permutations of specific cycle type we will use the fact that number of permutations of cycle type λ in group S_n is possible to get by a formula [9]:

$$k_\lambda = \frac{n!}{i_1^{p_1} p_1! i_2^{p_2} p_2! \dots i_m^{p_m} p_m!}, \tag{14}$$

where p_k is the number of elements i_k in λ.
As $I = I' = J'$ all permutations σ^{-1} such that $\sigma \in S$ according to definition permutes multiindices I' into I and since $I' = J'$ all such permutations have equal product on J'. Then reduced set of permutations S' (defined in section 3.1.) contains only one element. Set S' can contain any permutation from S and since identity permutation e belongs to set S we can define $S' = \{e\}$ in order to simplify further computation.

Now when set S' contains only identity permutation summation over all products of inversions of permutations from S' and permutations from T is equivalent to summation over set T. According to the fact that permutations from T are products of permutations of blocks of multiindices J we can write a formula:

$$\begin{aligned}
&\int U_{i_1,j_1} \dots U_{i_n,j_n} \overline{U_{i'_1,j'_1} \dots U_{i'_n,j'_n}} \mathrm{d}U = \\
&l_1! \cdot \dots \cdot l_k! \sum_{\tau_1 \in S_{l_1}, \dots, \tau_k \in S_{l_k}} Wg(\tau_1 \cdots \tau_k, n, d) = \\
&l_1! \cdot \dots \cdot l_k! \sum_{\lambda_1 \vdash l_1, \dots, \lambda_k \vdash l_k} k_{\lambda_1} \cdots k_{\lambda_k} Wg(\lambda_1 \sqcup \dots \sqcup \lambda_k, n, d).
\end{aligned} \tag{15}$$

Using formula above computation of integral is reduced to computing all partitions of lengths of blocks in multiindices J instead of computing all possible permutations and counting theirs cycle types.

3.4. Special case 3: general block diagonal matrices

When monomial contains elements that can be divided into blocks size $l_1, l_2, \dots, l_k$ then lists of indices also can be divided into the same blocks. Thus permutations I into I' and J into J' are products of disjoint permutations of indices in every block independently. When blocks in permutations from S and T are the same then products of permutations $\tau\sigma^{-1}, \tau \in T, \sigma \in S$ contains the same blocks. Because of this, problem of counting all products of permutations length d can be simplified to counting permutations which lengths are equal to dimensions of blocks.

$$N(\lambda) = \sum_{\substack{\lambda_1 \vdash l_1, \dots, \lambda_k \vdash l_k \\ \lambda_1 \sqcup \lambda_2 \sqcup \dots \sqcup \lambda_k = \lambda}} N_1(\lambda_1) \cdot \dots \cdot N_k(\lambda_k) \tag{16}$$

After applying this formula to general computation formula (9) following equation occurs:

$$\int U_{i_1,j_1}\dots U_{i_n,j_n}\overline{U_{i'_1,j'_1}\dots U_{i'_n,j'_n}}\mathrm{d}U = \sum_{\lambda\vdash n} N(\lambda)Wg(\lambda,n,d) =$$

$$\sum_{\lambda_1\vdash l_1,\dots,\lambda_k\vdash l_k} N_1(\lambda_1)\cdot\ldots\cdot N_k(\lambda_k)Wg(\lambda,n,d). \tag{17}$$

Using formula above it is still necessary to obtain some permutations but instead of computing permutations from group S_d it is possible to work on permutations from smaller groups $S_{l_1}, S_{l_2}, \dots, S_{l_k}$.

4. Applications of the integral

One can use integration unitary in number of sciences. It is an important subject of studies in many areas of science where polynomial functions of elements of unitary matrices are discussed. In this section we present examples of appliances.

4.1. MIMO channels

MIMO(Multi Input Multi Output) is a technology in radio channels based on use of multiple antennas at both the transmitter and receiver In this paper it has been studied in context of analysis key parameters of MIMO channels.

The time-invariant channel is described by [10]:

$$y = Hx + w, \tag{18}$$

where H is an Hermitian matrix. Matrix H has a Singular Value Decomposition (SVD):

$$H = U\Delta V^*, \tag{19}$$

where U, V are unitary matrices. The SVD decomposition of matrix H can be interpreted as coordinate transformations of input and output values. Such interpretation leads to angular domain representation of signals where

$$x^a := U_t^* x, \tag{20}$$

$$y^a := U_r^* y. \tag{21}$$

Thus calculating average values of signals or H matrix includes integration unitary.

Integrates of polynomial function are also important to computing correlation between path gains Correlation coefficients between signals transmitted by jth antenna and kth antenna depends on expectation values of elements of matrix H [11]. Thus to study correlation between Path Gains one need to compute estimated value of elements of H and its products. Due to SVD of H averaging H is reduced to problem of averaging monomials of elements of unitary matrices.

4.2. Quantum transport

In this section we consider applications of integration unitary connected with quantum transport. We consider a phase-coherent conduction through a chaotic cavity and through the interface between a normal metal and a superconductor [12]. In both discussed applications we obtain the conductance as a rational function of a unitary matrix.

First let us consider a system consisting of a chaotic cavity attached to two leads, containing tunnel barriers. The conductance G is a function of trace of some matrix S. Matrix S is distributed according to the circular ensemble. By using matrix decomposition of δS the problem of averaging S with Poisson kernel can be reduced to integrating matrix U that occurs in this decomposition over the unitary group.

Very similar reasoning track can be done while analysis average conductance of a system. Average conductance is given by a Landauer formula and using the same decomposition it can be reduced to the problem of integration unitary. Conductance fluctuations are considered as covariance of the conductance thus all computation can be done very similarly.

In order to introduce another application for integration unitary we consider a junction between a normal metal and a superconductor (NS junction). Using the relationship between the differential conductance of the NS junction [13, 14] and some transmission and reflection matrices one can obtain the conductance formula involving some unitary matrix function. Averages of conductance is computed in two steps and the first one is integration over unitary matrix [12]. Since conductance fluctuations are computed as variance of conductance, it involves first moment of conductance and is computed the same way.

5. Summary

We described practical and efficient methods for calculating integrals of polynomial functions of unitary matrices over the unitary group with respect to the Haar measure. We developed a technique for general case of any polynomial function. We also presented some special cases of functions and proper methods of computing integrals of such functions. As applications of integrating unitary matrices we introduced issues of quantum transport and MIMO channels.

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Efektywne metody całkowania wielomianów na grupie macierzy unitarnych względem miary Haara z zastosowaniami

Streszczenie

W pracy przedstawione zostały efektywne algorytmy całkowania funkcji wielomianowych na grupie macierzy unitarnych względem miary Haara. Przywołana została formuła Collinsa-Sniadego służąca do obliczania rozpatrywanej całki. Następnie rozpatrzono możliwości przyśpieszenia obliczeń prezentując efektywny algorytm. Pokazano szczególne przypadki rodzin wielomianów, dla których wartość całki może być wyznaczona analitycznie. Zostały również przywołane przykłady zastosowań całkowania wielomianów macierzy unitarnych w różnych działach nauki.