Symbolic integration with respect to the Haar measure on the unitary groups

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Abstract. We present IntU package for Mathematica computer algebra system. The presented package performs a symbolic integration of polynomial functions over the unitary group with respect to unique normalized Haar measure. We describe a number of special cases which can be used to optimize the calculation speed for some classes of integrals. We also provide some examples of usage of the presented package.

Key words: unitary group, Haar measure, circular unitary ensemble, symbolic integration

1. Introduction

The integration over unitary group is an important subject of studies in many areas of science, including mathematical physics, random matrix theory and algebraic combinatorics. In 2006 Collins and Śniady [1] proved a formula for calculating polynomial integrals over U(d). In [2] they showed some examples of the usage. In Section 6 we provide a package with the list of main functions. In Section 5 we introduce notation present mathematical background concerning polynomial integrals over U(d) with respect to the Haar measure. We describe a number of special cases which can be used to optimize the calculation speed for some classes of integrals. We also provide some examples of usage of the presented package including the applications in the study of the geometry of the quantum states.

This paper is organised as follows. In Section 2 we introduce notation present mathematical background concerning polynomial integrals over unitary group. In Section 3 we describe some special cases, in which the integration can be calculated more efficiently. In Section 4 we provide the description of the IntU package with the list of main functions. In Section 5 we show some examples of the usage. In Section 6 we provide a summary of the presented results and give conclusions.

2. Mathematical background

2.1. Basic concepts

We denote by Mn square matrices of size n. The compact group of d × d unitary matrices we denote as U(d). We equip the above group with unique normalized Haar measure denoted by dU. Random elements distributed with measure dU form so called Circular Unitary Ensemble.

Integer partition λ of a positive integer n is a weakly decreasing sequence λ = (λ1, λ2, . . . , λl) of positive integers, such that ∑l1=1 λi = |λ| = n. To denote that λ is a partition of n we write λ ↑ n. The length of a partition is denoted by l(λ). By λ ↑ µ we denote a partition of n1 + n2 obtained by joining partitions λ ↑ n1 and µ ↑ n2.

Each permutation σ ∈ Sn can be uniquely decomposed into a sum of disjoint cycles where the lengths of the cycles sum up to n. Thus the vector of the lengths of the cycles, after reordering, forms a partition λ ↑ n. The partition λ is called the cycle type of permutation σ.

2.2. Moments of the U(d)

Let us consider a polynomial p. From the linearity of an integral we have

\[ \int_{U(d)} p(U) dU = \sum_{I, J, I', J'} c(I, J, I', J') \int_{U(d)} U_{IJ} U_{I'J'} dU, \]  

where I, J, I', J' are multi-indices and c are the coefficients of p. The value of such monomial integrals is given as

\[ \int_{U(d)} U_{IJ} U_{I'J'} dU = \int_{U(d)} U_{I1J1} \ldots U_{I'nJ'n} dU = \sum_{\sigma, \tau \in S_n} \delta_{\sigma_{I1} \tau_{I1}} \delta_{\sigma_{I2} \tau_{I2}} \ldots \delta_{\sigma_{I'n} \tau_{I'n}} Wg(\tau \sigma^{-1}, d), \]  

where Wg is the Weingarten function discussed below. In the case where the multi-indices differ in length, i.e. n ≠ n', we have

\[ \int_{U(d)} U_{IJ} U_{I'J'} dU = \int_{U(d)} U_{I1J1} \ldots U_{I'nJ'n} dU = 0. \]  

The integrals of the above type are known as moments of the U(d).

2.3. Weingarten function

The Weingarten function [11] is defined for σ ∈ Sn and positive integer d, as

\[ Wg(\sigma, d) = \frac{1}{(n!)^2} \sum_{\lambda | \lambda \vdash d} \chi^\lambda (\sigma) s_{\lambda, d}(1) \chi^\lambda (\sigma), \]

where the sum is taken over all integer partitions of n with length l(λ) ≤ d, sλ,d(1) is the Schur polynomial sλ evaluated...
at \((1,1,\ldots,1)\) and \(\chi^\lambda\) is an irreducible character of the symmetric group \(S_n\) indexed by partition \(\lambda\).

2.3.1. The dimension of irreducible representation of \(U(d)\)

The value of the Schur polynomial at the point \((1,1,\ldots,1)\), \(i.e.\) the dimension of irreducible representation of \(U(d)\) corresponding to partition \(\lambda\), is equal to (see \(e.g.\) \([5]\) Theorem 6.31)

\[
s_{\lambda,d}(1) = s_{\lambda}(1,1,\ldots,1) = \prod_{1 \leq i < j \leq d} \frac{\lambda_i - \lambda_j + j - i}{j - i}.
\]

2.3.2. Irreducible character of \(S_n\)

The irreducible character of \(S_n\) indexed by partition \(\lambda\), \(\chi^\lambda(\sigma)\) depends on a conjugacy class of permutation \(\sigma\). Two permutations are in the same conjugacy class if and only if they have the same cycle type, thus it is common to write \(\chi^\lambda(\sigma) = \chi^\lambda(\mu)\), where \(\mu\) is an integer partition corresponding to the cycle type of \(\sigma\).

In the case of identity permutation the cycle type is given by a trivial partition, \(e = (1,1,\ldots,1)\), and the character value is equal to the dimension of the irreducible representation of \(S_n\) indexed by \(\lambda\). In this case it is given by the celebrated hook length formula \([5]\) Eq. 4.12

\[
\chi^\lambda(e) = \frac{|\lambda|!}{\prod_i h^\lambda_{i,i}},
\]

where \(|\lambda| = \lambda_1 + \lambda_2 + \ldots + \lambda_n\), and \(h^\lambda_{i,i}\) is the hook length of the cell \((i,i)\) in a Ferrers diagram corresponding to partition \(\lambda\), see \(e.g.\) \([6]\) p. 57).

In the case of a non-trivial partition the character of symmetric group \(\chi^\lambda(\sigma) = \chi^\lambda(\mu)\) can be evaluated with the use of Murnaghan-Nakayama rule (see \(e.g.\) \([7]\) Th. 4.10.2)), which describes a combinatorial way of calculating the character. \([9]\) is used.

From the above considerations one can notice that the Weingarten function depends only on a cycle type of a permutation \(\sigma\) and thus it is constant on a conjugacy class represented by \(\sigma\). Thus we may define the Weingarten function as

\[
W_{\mu}(\mu,d) = \frac{1}{(|\mu|)!^3} \sum_{\lambda:|\lambda| = |\mu|} \frac{\chi^\lambda(\mu)^2}{s_{\lambda,d}(1)} \chi^\lambda(\mu),
\]

where \(\mu\) is an integer partition, which is a cycle type of \(\sigma\).

3. Special cases

In this section we present some special cases of integrals, with respect to the Haar measure on the unitary group. In these cases the value of the integral can be calculated without the direct usage of formula \([3]\), which requires processing of \(\prod_k k! \prod_j l_j!\) permutations, where \(k_i (l_j)\) denotes the number of \(i\) (\(j\)) in multi-indices \(I\) (\(J\)) respectively.

The presented special cases have been implemented in the package, to increase its efficiency. This goal has been achieved by minimizing the number of calculations of the Weingarten function.

3.1. First two moments of \(U(d)\)

In the case of monomials of rank equal to 2 and 4, we have \([9]\) Prop. 4.2.3] formulas

\[
\int_{U(d)} u_{i_1} \delta_{i_1,f} dU = \frac{1}{d-1} \delta_{i_1,f},
\]

and

\[
\int_{U(d)} u_{i_1} u_{j_1} u_{i_2} u_{j_2} \delta_{i_1,f} \delta_{j_2,f} dU = \frac{1}{d-1} \delta_{i_1,f} \delta_{j_2,f} \delta_{i_2,f} \delta_{j_1,f} + \frac{1}{d-2} \frac{1}{d-1} \delta_{i_1,f} \delta_{j_2,f} \delta_{i_2,f} \delta_{j_1,f} + \frac{1}{d-2} \frac{1}{d-1} \delta_{i_1,f} \delta_{j_1,f} \delta_{i_2,f} \delta_{j_2,f},
\]

allowing calculation of the values for polynomial integrals of degree less than 5 without the direct usage of the formula \([3]\).

This optimization gives only a minor improvement of efficiency, as in these cases the direct calculation of Weingarten function is very fast.

3.2. Elements from one row (column)

The next optimization is based on the fact that the distribution of random vector consisting of squares of absolute values of a row (or a column) of unitary matrix distributed with the Haar measure, is uniform on a standard \(d\)-simplex \(\Delta^d\) \([9]\) Ch. 4]

\[
\{ |u_{i_1}|^2, |u_{i_2}|^2, \ldots, |u_{i_d}|^2 \} \sim \mathbb{U}(\Delta^d),
\]

where \(\mathbb{U}(A)\) denotes the normalized uniform measure (proportional to Lebesgue measure) on a set \(A \subset \mathbb{R}^d\), and standard \(d\)-simplex \(\Delta^d\) is defined as, \(\Delta^d = \{ \lambda \in \mathbb{R}^d : \lambda_i \geq 0, \sum_{i=1}^d \lambda_i = 1\}\).

Using Beta integral, one obtains that for a fixed row \(i\) and a vector \(p\) with non-negative entries \(p_j\), we have the following

\[
\int_{U(d)} \prod_{j=1}^d |u_{i,j}|^{2p_j} dU = \Gamma(d) \frac{\Gamma((p_1 + 1) \times \cdots \times \Gamma((p_d + 1))}{\Gamma(p_1 + \cdots + p_d + d)},
\]

The above, as a special case, gives us:

\[
\int_{U(d)} |u_{i,j}|^{2k} dU = \frac{(d-1)!k!}{(d-1+k)!},
\]

\[
\int_{U(d)} |u_{i,j}|^{2k} |u_{k,l}|^{2d} dU = \frac{1}{d(d+1)},
\]

which can be found in literature \([9]\), \([10]\).

This optimization allows for an enormous improvement in efficiency thanks to avoiding \(\{ \sum p_i \}| \prod p_i \} \) executions of Weingarten function needed in the case of the direct usage of formula \([3]\).

3.3. Even powers of diagonal element absolute values

In this subsection we consider the integrals of the type

\[
\int_{U(d)} |u_{i,j}|^{2p} |u_{k,l}|^{2q} dU,
\]

which can be found in literature \([9]\), \([10]\).
where \( p, q \) are non-negative integers and \( i \neq k, j \neq l \). In the case of \( p = q = 1 \) this integral is known \([9]\) Prop. 4.2.3
\[
\int_{U(d)} |u_{ij}|^2 |u_{kl}|^2 dU = \frac{1}{d^2 - 1}.
\tag{16}
\]
For general non-negative integers \( p, q \) the following proposition is true.

**Proposition 1.** Let \( p, q \) be non-negative integers, for \( i \neq k \) and \( j \neq l \), we have
\[
\int_{U(d)} |u_{ij}|^2 |u_{kl}|^2 dU = p!q! \sum_{\lambda \vdash p} \sum_{\mu \vdash q} k_\lambda k_\mu W_{\lambda \mu} (\lambda \sqcup \mu, d),
\tag{17}
\]
where the above sum is taken over all integer partitions of \( p \) and \( q \). Symbol \( k_\lambda \) denotes a cardinality of conjugacy class for a permutation with cycle type given by partition \( \nu \vdash r \) \([7]\) Eq. 1.2
\[
k_\nu = \frac{r!}{m_1! m_2! m_3! \cdots m_r!},
\tag{18}
\]
where \( m_i \) denotes the number of \( i \) in partition \( \nu \).

The above is a special case of a more general fact.

**Proposition 2.** For any permutation \( \pi \in S_d \) and any non-negative integers \( p_1, p_2, \ldots, p_d \), we have
\[
\int_{U(d)} \prod_{j=1}^d |u_{j, \pi(j)}|^{2p_j} dU = \int_{U(d)} \prod_{j=1}^d |u_{ij}|^{2p_j} dU =
\]
\[
= \left( \prod_{j=1}^d p_j! \right) \sum_{\lambda_1 \vdash p_1} \sum_{\lambda_2 \vdash p_2} \cdots \sum_{\lambda_d \vdash p_d} \left( \prod_{j=1}^d k_{\lambda_j} \right) \times W_{\lambda_1 \sqcup \lambda_2 \sqcup \cdots \sqcup \lambda_d} (\lambda_1 \sqcup \lambda_2 \sqcup \cdots \sqcup \lambda_d, d).
\tag{19}
\]

**Proof.** If we apply the formula from Eq. \((9)\) to integral \((19)\), then the non-vanishing permutations of indices are those which permute within the blocks of sizes \( \{p_1, p_2, \ldots, p_d\} \), i.e.
\[
\sigma = \sigma_1 \oplus \sigma_2 \oplus \cdots \oplus \sigma_d,
\]
where \( \sigma_j \in S_{p_j} \) and it permutes indices in \( j \)-th block of size \( p_j \). The same situation holds in the case of the second indices. Thus the permutation \( \tau \sigma^{-1} \) is also in this form. Each permutation of the above type will be present in the sum \( \prod_{j=1}^d p_j! \) times. The cycle type of such permutations is given by a partition which is obtained by joining cycle types of small permutations. Since Weingarten function depends only on a cycle type of permutation, the size of conjugacy class is calculated for each partition, instead of evaluating multiple times Weingarten function. \[\square\]

The formula \((19)\) is far less computationally demanding than the direct usage of \((9)\). One can notice that Proposition \((2)\) allows us to avoid at least \( \prod_{j=1}^d p_j! \) executions of Weingarten function comparing to the direct usage of \((9)\). However, the exact time-efficiency depends also on the cardinality of conjugacy classes for partitions of \( p_1, \ldots, p_d \).

### 3.4. Cycle permutations

In this section we consider another special type of integral for positive integer \( k \) and a permutation \( \sigma \in \{1, 2, \ldots, m\} \) being a cycle
\[
\int_{U(d)} \left( \prod_{j=1}^m u_{ij, \sigma(i)} \right)^k dU.
\tag{20}
\]

We have the following proposition.

**Proposition 3.** Let \( m \leq d \), \( k \) is a positive integer and \( \sigma \in S_m \) be a cycle, i.e. the cycle type is given by partition \( \{m\} \). Then
\[
\int_{U(d)} \left( \prod_{j=1}^m u_{ij, \sigma(i)} \right)^k dU = (k!)^{2m-1} \sum_{\lambda \vdash k} k_\lambda W_{\lambda m} (m\lambda, d).
\tag{21}
\]

**Proof.** One can notice that cycle lengths of permutations in this setting must be divisible by \( m \). The number of permutations with cycle type given by a particular partition can be easily obtained by the usual counting argument. \[\square\]

Using the above formula \((21)\) one obtains an enormous improvement in efficiency by avoiding more than \( (k!)^{2m-1} \) executions of Weingarten function, comparing to the case of the direct usage of \((9)\).

### 4. Package description

Below we describe the functions implemented in \texttt{IntU} package. The functions are grouped in three categories: functions implementing the main functionality, functions related to the calculation of Weingarten function and helper functions.

#### 4.1. Main functionality

The main functionality of \texttt{IntU} package is provided by the \texttt{IntegrateUnitaryHaar} and \texttt{IntegrateUnitaryHaarIndices} functions. The first one operates directly on polynomial expressions, while the second one accepts four-tuple of indices. The examples of the usage are given in Section 5

- \texttt{IntegrateUnitaryHaar\{integrand,\{var,dim\}\}} – gives the definite integral on unitary group with respect to the Haar measure, accepting the following arguments
  - \texttt{integrand} – the polynomial type expression of variable \( \texttt{var} \) with indices placed as subscripts, can contain any other symbolic expression of other variables,
  - \texttt{var} – the symbol of variable for integration,
  - \texttt{dim} – the dimension of a unitary group, must be a positive integer.

This function is presented in the examples described in Sections \(5.1\), \(5.3\) and \(5.5\).

- \texttt{IntegrateUnitaryHaar\{f,\{u,d1\},\{v,d2\},\ldots\}} – gives multiple integral
  \[
  \int_{U(d1)} dU \int_{U(d2)} dV \ldots f.
  \tag{22}
  \]

This function is presented in the example described in Section 5.4.
5. Usage examples

In order to present the main features of the described package we provide a series of examples.

5.1. Elementary integrals

Let us assume that \( d = 3 \). We want to calculate the following integrals

\[
\int_{U(d)} \left| u_{1,1} \right|^2 dU, \quad \int_{U(d)} \left| u_{1,1} \right|^2 \left| u_{2,2} \right|^2 dU, \quad \int_{U(d)} u_{1,1} u_{2,2} \bar{u}_{1,2} \bar{u}_{2,1} dU.
\]

Let us start by initializing the package

```math
\text{In}[1] = \text{<< IntU`}
```

```math
\text{In}[2] = d = 3;
```

```math
\text{In}[3] = \text{IntegrateUnitaryHaar[}
\text{Abs}[u_{1,1}] \wedge 2, \{u, d\}]
```

```math
\text{Out}[3] = \frac{1}{3}
```

```math
\text{In}[4] = \text{IntegrateUnitaryHaar[}
\text{Abs}[u_{1,1} u_{2,2}] \wedge 2, \{u, d\}]
```

```math
\text{Out}[4] = \frac{1}{8}
```

```math
\text{In}[5] = \text{IntegrateUnitaryHaar[u_{1,1} u_{2,2}]
\text{Conjugate}[u_{1,2} u_{2,1}], \{u, d\}]
```

```math
\text{Out}[5] = \frac{1}{24}
```

5.2. Operations on indices

Let us take the following set of multi-indices

\[
I = \{1, 1, 1, 2, 2\}, \quad J = \{2, 2, 1, 1, 1\}
\]

\[
I' = \{1, 1, 1, 2, 2\}, \quad J' = \{2, 1, 1, 2\}
\]

and set \( d = 6 \). The above is equivalent to expression

\[
u_{1,2} u_{1,1} u_{2,1} u_{2,2} \bar{u}_{1,1} \bar{u}_{1,2} \bar{u}_{2,1} \bar{u}_{2,2}.
\]

with symbolic variable \( \alpha \), which we aim to integrate over \( U(d) \).

After simplification the expression is equal to

\[
\left| u_{1,1} \right|^2 \left| u_{1,2} \right|^2 \left| u_{2,2} \right|^2 u_{1,2} u_{2,1} \bar{u}_{1,1} \bar{u}_{2,2}.
\]

After initializing the package and defining appropriate indices

```math
\text{In}[2] = \text{II} = \{1, 1, 1, 2, 2\}; \quad J1 = \{2, 2, 1, 1, 1\};
\text{II} = \{1, 1, 1, 2, 2\}; \quad J2 = \{2, 1, 1, 1, 2\};
\text{d} = 6;
```

we calculate the integral using provided function

```math
\text{IntegrateUnitaryHaarIndices as}
```
5.3. Matrix expressions

The IntU package allows us to integrate matrix expressions, for example let us take $d = 2$ and integrate

$$
\int_{U(d)} U^\otimes 2 \otimes \bar{U}^\otimes 2 dU.
$$

We define symbolic matrices $U \in U(d)$ and $U^2 = U \otimes U \in U(2d^2)$ as

$$
U = \text{Array}[u_{ij}, 2, 2],
$$

and construct the integrand as

$$
\text{integrand} = \text{KroneckerProduct}[U^2, \text{Conjugate}[U^2]].
$$

By using IntegrateUnitaryHaar function

$$
\text{IntegrateUnitaryHaar}[
\text{integrand}, \{u, d\}
$$

we learn that the integral in Eq. (31) is equal to

$$
\frac{1}{16 \cdot 200}
$$

5.4. Mean value of local unitary orbit

In this example we calculate the mean value of a local unitary orbit of a given matrix $X \in M_{d^2}$

$$
E[(U \otimes V)X(U \otimes V)^\dagger].
$$

We assume that $U$ and $V$ are stochastically independent random unitary matrices of size $d$ distributed with the Haar measure. In this case we have

$$
E[(U \otimes V)X(U \otimes V)^\dagger] = \int_{U(d)} \int_{U(d)} (U \otimes V)X(U \otimes V)^\dagger dUdV.
$$

In this example we take $d = 3$. We define symbolic matrices $X$ of size $d^2$ and $U,V \in U(d)$ as

$$
X = \text{Array}[x_{ij}, 3, 3],
$$

and construct the integrand as

$$
\text{integrand} = \text{KroneckerProduct}[U^2, \text{Conjugate}[U^2]].
$$

By using IntegrateUnitaryHaar function

$$
\text{IntegrateUnitaryHaar}[
\text{integrand}, \{u, d\}
$$

we learn that the integral in Eq. (34) is equal to

$$
\frac{1}{16 \cdot 200}
$$

5.5. Moments of maximally entangled numerical shadow

If $U$ is a random $d \times d$ unitary matrix distributed according to the Haar measure \cite{12} then the pure state obtained by vectorization $|\xi\rangle = \frac{1}{\sqrt{d}} \text{vec}(U)$ is maximally entangled on $H_A \otimes H_B = \mathbb{C}^d \otimes \mathbb{C}^d$. Moreover, state $|\xi\rangle$ has a distribution invariant to multiplication by local unitary matrices. We denote the corresponding probability measure on pure states of size $d \times d$ as $\mu$. The numerical shadow of operator $X \in M_{d^2}$ with respect to this measure (maximally entangled numerical shadow) is defined as

$$
P_X(z) = \int_{\mathbb{C}^d} \delta(z - (\psi|X|\psi)) d\mu(\psi).
$$

The corresponding probability measure is denoted by $d\mu^\xi$. For definition and basic facts concerning numerical shadows see \cite{11, 13, 14}.

The first two moments of $d\mu^\xi$ are calculated in \cite{11}, and are given by

$$
\int \bar{z} d\mu^\xi(z) = \frac{1}{d^2} \text{tr} X,
$$

and

$$
\int \bar{z} z d\mu^\xi(z) = \frac{1}{d^2(d^2-1)} \left( |\text{tr} X|^2 + \|X\|_{\text{HS}}^2 \right) - \frac{1}{d^2(d^2-1)} \left( |\text{tr}_A(X)|_{\text{HS}}^2 + |\text{tr}_B(X)|_{\text{HS}}^2 \right),
$$

where $\text{tr}_A$ and $\text{tr}_B$ denote partial traces over a specified sub-system and $\| \cdot \|_{\text{HS}}$ is a Hilbert-Schmidt norm given by $\|X\|_{\text{HS}} = \sqrt{\text{tr}(XX^\dagger)}$.

In order to calculate Eqs. (39) and (39) define symbolic matrices...
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6. Summary
We described IntU package for Mathematica computing system for calculating polynomial integrals over $U(d)$ with respect to Haar measure. We described some number of special cases which can be used to optimize the calculation speed for some classes of integrals. We also provide some examples of the usage of the presented package including the applications in the geometry of the quantum states.

Calculation time of the package strongly depends on a degree of the integrand. For polynomials of small degree the package is able to calculate the value of integral using the direct formula \[\text{(3)}\]. For polynomials of large degree the calculation time grows rapidly and the calculation is possible only if one of the special cases (optimizations) is used.

Nevertheless, the presented package can be very useful in the investigations involving Circular Unitary Ensemble and the geometry of quantum states and quantum entanglement.

7. Acknowledgements
Work of Z. Puchała was partially supported by the Polish National Science Centre under the research project N N514 513340 while work of J. A. Miszczak was partially supported by the Polish National Science Centre under the research project N N516 475440. Authors would like to thank K. Życzkowski and P. Gawron for motivation and interesting discussions.

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