Composite parameterization and Haar measure for all unitary and special unitary groups

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QFGI 2013 // 04.04.2013

Outline

Composite parameterization and Haar measure for all unitary and special unitary groups

Common (optimization) problems in quantum information

- separability problem:
  - optimize $Q(U_{local}\rho U_{local}^{\dagger})$ over all $U_{local} = U_1 \otimes \ldots \otimes U_n$
- optimal measurement setting for Bell tests:
  - maximize $I = Tr\,(\rho\mathcal{B})$ over all local observables
- distillability of quantum states:
  - seek entangled $\mathbb{C}^2 \otimes \mathbb{C}^2$ subsystem
- features related to the rank k of a density matrix ρ
- generate (unbiased) random unitaries, states and subspaces
  - Monte Carlo simulations, Data Hiding
- compute group integrals $\int f(U)dU$
  - Werner and isotropic states
  - *A priori* (average) entanglement $\overline{E} = \int E(|\psi\rangle)d\psi$

Consider a d-dimensional complex Hilbert space $\mathcal{H} = \mathbb{C}^d$

How to parameterize?

- unitary matrices
- set of k orthonormal vectors
- density matrices of rank k
- k-dimensional subspaces (Grassmannians $\mathrm{Gr}(k, \mathbb{C}^d)$)

Requirements

- efficient and redundancy-free
- easy to implement
- insightful
- computationally inexpensive

Popular parameterizations:

Canonical parameterization of $\mathcal{U}(d)$ and $\mathcal{SU}(d)$

$$U = \exp(iH) \qquad H - \text{hermitian (and traceless for } \mathcal{SU}(d))$$

Euler angle parameterization of $\mathcal{U}(d)$ and $\mathcal{SU}(d)$

$$U = \prod_{n=1}^{d^2-1} \exp\left(i\Lambda_{f(n)}\alpha_n\right) \qquad (\times \exp(i\alpha_{d^2}) \text{ for } \mathcal{U}(d))$$

Infinitesimal generators: $d^2 - 1$ **Generalized Gell-Mann Matrices** (GGM)

- $\frac{d(d-1)}{2}$ symmetric GGM matrices
  $\Lambda^s_{m,n} = |m\rangle\langle n| + |n\rangle\langle m| \qquad 1 \le m < n \le d$
- $\frac{d(d-1)}{2}$ antisymmetric GGM matrices
  $\Lambda^a_{m,n} = -i\,|m\rangle\langle n| + i\,|n\rangle\langle m| \qquad 1 \le m < n \le d$
- $(d-1)$ diagonal GGM matrices
  $\Lambda_n = \sqrt{\frac{2}{n(n+1)}}\left(\sum_{j=1}^{n} |j\rangle\langle j| - n\,|n+1\rangle\langle n+1|\right) \qquad 1 \le n \le d-1$

Idea: compose the unitary group $\mathcal{U}(d)$ out of 'elementary' operations

$$\textbf{rotations} \leftrightarrow \exp\left(iY_{m,n}\lambda\right) \qquad Y_{m,n} = -i\,|m\rangle\langle n| + i\,|n\rangle\langle m|$$

$$\textbf{phases} \leftrightarrow \exp\left(iP_{n}\lambda\right) \qquad P_{n} = |n\rangle\langle n|$$

Construction

Central characteristic of unitary operators: $\{|1\rangle, \ldots, |d\rangle\} \mapsto \{|1'\rangle, \ldots, |d'\rangle\}$

Step 1: d global phases $\{|1\rangle, \ldots, |d\rangle\} \mapsto \left\{e^{i\alpha_1}|1\rangle, \ldots, e^{i\alpha_d}|d\rangle\right\}$

$$U = \prod_{l=1}^{d} \exp(iP_l\lambda_{l,l})$$

Step 2: $\frac{d(d-1)}{2}$ distinctive operations $\Lambda_{m,n} = \underbrace{\exp\left(iP_n\lambda_{n,m}\right)}_{\text{relative phase}}\ \underbrace{\exp\left(iY_{m,n}\lambda_{m,n}\right)}_{\text{rotation}}$

$$U = \prod_{m=1}^{d-1}\left(\prod_{n=m+1}^{d} \exp\left(iP_n\lambda_{n,m}\right)\exp\left(iY_{m,n}\lambda_{m,n}\right)\right)$$

Composite parameterization of $\mathcal{U}(d)$

$$U_C = \left[\prod_{m=1}^{d-1}\left(\prod_{n=m+1}^{d}\exp\left(iP_n\lambda_{n,m}\right)\exp\left(iY_{m,n}\lambda_{m,n}\right)\right)\right]\cdot\left[\prod_{l=1}^{d}\exp(iP_l\lambda_{l,l})\right],$$

$[d \times d]$ **parameter matrix:**

$$\text{relative phases} \rightarrow \begin{pmatrix} \lambda_{1,1} & \cdots & \lambda_{1,d} \\ \vdots & \ddots & \vdots \\ \lambda_{d,1} & \cdots & \lambda_{d,d} \end{pmatrix} \leftarrow \text{rotations}$$

ranges : $\lambda_{m,n} \in [0, 2\pi]$ for $m \geq n$ $\quad \lambda_{m,n} \in \left[0, \frac{\pi}{2}\right]$ for $m < n$

Proof: $\forall U \in \mathcal{U}(d)$ $\quad \exists U_C$ such that $U = U_C$

arbitrary $U = \sum_{r,s=1}^{d} a_{r,s} \left|r\right\rangle \left\langle s\right|$ $\quad \Leftrightarrow \quad \sum_{i=1}^{d} a^*_{m,i}a_{n,i} = \sum_{i=1}^{d} a^*_{i,m}a_{i,n} = \delta_{mn}$

$$U_C^{\dagger}U \stackrel{!}{=} \mathbb{1}$$

$$U_C^\dagger U = \left[\prod_{l=1}^{d} \exp(-iP_{d+1-l}\lambda_{d+1-l,d+1-l})\right] \left[\prod_{m=1}^{d-1}\left(\prod_{n=1}^{m}\Lambda^\dagger_{d-m,d+1-n}\right)\right] U$$

For $U' = \Lambda^\dagger_{1,2}U = \sum_{r,s=1}^{d} a'_{r,s}\,|r\rangle\langle s|$ this leads to (row transformation)

$$a'_{1,s} = \cos(\lambda_{1,2})a_{1,s} - e^{-i\lambda_{2,1}}\sin(\lambda_{1,2})a_{2,s}\ ,$$
$$a'_{2,s} = \underbrace{\sin(\lambda_{1,2})a_{1,s}}_{\text{abs. value}} + \underbrace{e^{-i\lambda_{2,1}}}_{\text{contrary argument}} \underbrace{\cos(\lambda_{1,2})a_{2,s}}_{=\text{abs. value}}\ .$$

$$\begin{array}{c}\exists\ \lambda_{1,2} \in [0, \frac{\pi}{2}] \\ \exists\ \lambda_{2,1} \in [0, 2\pi)\end{array} \quad \Rightarrow\ U' = \begin{pmatrix} \star & \star & \star & \star \\ 0 & \star & \star & \star \\ \star & \star & \star & \star \\ \star & \star & \star & \star \end{pmatrix}$$

$$\ldots \prod_{m=1}^{d-1}\left(\prod_{n=1}^{m}\Lambda^\dagger_{d-m,d+1-n}\right) U = \begin{pmatrix} \star & 0 & 0 & 0 \\ 0 & \star & 0 & 0 \\ 0 & 0 & \star & 0 \\ 0 & 0 & 0 & \star \end{pmatrix}$$

$$\ldots \left[\prod_{l=1}^{d} \exp(-iP_{d+1-l}\lambda_{d+1-l,d+1-l})\right] \left[\prod_{m=1}^{d-1}\left(\prod_{n=1}^{m}\Lambda^\dagger_{d-m,d+1-n}\right)\right] U = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$\square$

II.1 Composite parameterization of $\mathcal{SU}(d)$

Replace: $\exp(i\lambda P_n) \rightarrow \exp(i\lambda Z_{m,n})$ $\qquad Z_{m,n} = |m\rangle\langle m| - |n\rangle\langle n|$

Composite parameterization of $\mathcal{SU}(d)$

$$U_C = \left[\prod_{m=1}^{d-1}\left(\prod_{n=m+1}^{d} \exp(iZ_{m,n}\lambda_{n,m})\exp(iY_{m,n}\lambda_{m,n})\right)\right]\cdot\left[\prod_{l=1}^{d-1}\exp(iZ_{l,d}\lambda_{l,l})\right]$$

$[d \times d] - 1$ **parameter matrix:**

$$\text{relative phases} \rightarrow \begin{pmatrix} \lambda_{1,1} & \cdots & \lambda_{1,d} \\ \vdots & \ddots & \vdots \\ \lambda_{d,1} & \cdots & \circ \end{pmatrix} \leftarrow \text{rotations}$$

ranges : $\lambda_{m,n} \in [0,\pi]$ for $m > n$ $\qquad \lambda_{m,n} \in \left[0, \frac{\pi}{2}\right]$ for $m < n$

$\lambda_{m,n} \in [0, 2\pi]$ for $m = n$

Consider an arbitrary set of k orthonormal vectors $\{|\Psi_1\rangle, \ldots, |\Psi_k\rangle\}$.
Any such set can be constructed via $\{U_C|1\rangle, \ldots, U_C|k\rangle\}$.

Construction of k orthonormal vectors with the minimal number of parameters

- The order of the operations $\Lambda_{m,n} = \exp(i\lambda_{n,m}P_n)\exp(i\lambda_{m,n}\sigma_{m,n})$ in

$$U_C = \left[\prod_{m=1}^{d-1}\left(\prod_{n=m+1}^{d}\exp(i\lambda_{n,m}P_n)\exp(i\lambda_{m,n}\sigma_{m,n})\right)\right]\left[\prod_{l=1}^{d}\exp(i\lambda_{l,l}P_l)\right]$$

  implies that $|\Psi_r\rangle = U_C|r\rangle$ is independent of all $\lambda_{m,n}$ with $m > r$ and $n > r$
- Diagonal entries $\lambda_{n,n}$ are physically irrelevant

parameter matrix :
$k(2d-k-1)$ parameters

$$\begin{array}{cc}
\underbrace{\begin{pmatrix}
0 & \lambda_{1,2} & \cdots & \lambda_{1,k+1} & \cdots & \lambda_{1,d} \\
\lambda_{2,1} & \ddots & \ddots & \vdots & \ddots & \vdots \\
\vdots & \ddots & 0 & \lambda_{k,k+1} & \cdots & \lambda_{k,d} \\
\lambda_{k+1,1} & \cdots & \lambda_{k+1,k} & 0 & \cdots & 0 \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
\lambda_{d,1} & \cdots & \lambda_{d,k} & 0 & \cdots & 0
\end{pmatrix}}_{\text{k} \qquad\qquad \text{d-k}} & \begin{array}{l} \left.\vphantom{\begin{array}{c}a\\a\\a\end{array}}\right\}\text{k} \\ \left.\vphantom{\begin{array}{c}a\\a\\a\end{array}}\right\}\text{d-k} \end{array}
\end{array}$$

II.3 Parameterization of density matrices of rank k

Consider an arbitrary density matrix of rank k on $\mathbb{C}^d$

$$\rho = \sum_{n=1}^{k} p_n \left|\Psi_n\right\rangle \left\langle\Psi_n\right| \qquad \Leftrightarrow \qquad \rho = \sum_{n=1}^{k} p_n U_C \left|n\right\rangle \left\langle n\right| U_C^{\dagger}$$

Parameterization of $\{p_1, \ldots, p_k\}$ with $k-1$ parameters $\theta_i \in [0, \frac{\pi}{2}]$

$$p_1 = cos^2\theta_1$$

$$p_n = cos^2\theta_n \prod_{i=1}^{n-1} sin^2\theta_i \qquad \forall n \ : \ 1 < n < k$$

$$p_k = \prod_{i=1}^{k-1} sin^2\theta_i$$

parameter matrix :
$k(2d-k-1)$ parameters

ρ with rank k :
$2dk - k^2 - 1$ parameters

$$\begin{array}{cc}
\begin{pmatrix}
0 & \lambda_{1,2} & \cdots & \lambda_{1,k+1} & \cdots & \lambda_{1,d} \\
\lambda_{2,1} & \ddots & \ddots & \vdots & \ddots & \vdots \\
\vdots & \ddots & 0 & \lambda_{k,k+1} & \cdots & \lambda_{k,d} \\
\lambda_{k+1,1} & \cdots & \lambda_{k+1,k} & 0 & \cdots & 0 \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
\lambda_{d,1} & \cdots & \lambda_{d,k} & 0 & \cdots & 0
\end{pmatrix}
&
\begin{array}{l}
\left.\vphantom{\begin{matrix} a \\ b \\ c \end{matrix}}\right\} \text{k} \\
\left.\vphantom{\begin{matrix} a \\ b \\ c \end{matrix}}\right\} \text{d-k}
\end{array}
\\
\underbrace{\hphantom{\lambda_{k+1,1} \quad \cdots \quad \lambda_{k+1,k}}}_{\text{k}} \quad \underbrace{\hphantom{\lambda_{k,k+1} \quad \cdots \quad \lambda_{k,d}}}_{\text{d-k}} &
\end{array}$$

II.4 Parameterization of k-dimensional subspaces in $\mathbb{C}^d$

Consider an arbitrary k-dimensional subspace spanned by the orthonormal vectors

$$|\Psi_1\rangle = \begin{pmatrix} a_{1,1} \\ \vdots \\ a_{d,1} \end{pmatrix}, \quad |\Psi_2\rangle = \begin{pmatrix} a_{1,2} \\ \vdots \\ a_{d,2} \end{pmatrix}, \quad \cdots \quad |\Psi_k\rangle = \begin{pmatrix} a_{1,k} \\ \vdots \\ a_{d,k} \end{pmatrix}$$

$$\begin{pmatrix} a_{1,1} & \cdots & a_{1,k} \\ \vdots & \ddots & \vdots \\ a_{d,1} & \cdots & a_{d,k} \end{pmatrix} \xrightarrow[\text{same subspace spanned by : (row transformations)}]{\text{linear combinations}} \begin{pmatrix} a'_{1,1} & \cdots & a'_{1,k} \\ 0 & \ddots & \vdots \\ 0 & 0 & a'_{k,k} \\ a'_{k+1,1} & \cdots & a'_{k+1,k} \\ \star & \star & \star \end{pmatrix}$$

parameter matrix :

$2k(d-k)$ parameters

$$\underbrace{\begin{pmatrix} 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0 \\ \lambda_{k+1,1} & \cdots & \lambda_{k+1,k} \\ \vdots & \ddots & \vdots \\ \lambda_{d,1} & \cdots & \lambda_{d,k} \end{pmatrix}}_{k} \!\!\!\! \underbrace{\begin{matrix} \lambda_{1,k+1} & \cdots & \lambda_{1,d} \\ \vdots & \ddots & \vdots \\ \lambda_{k,k+1} & \cdots & \lambda_{k,d} \\ 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0 \end{matrix}}_{\text{d-k}} \begin{matrix} \left.\vphantom{\begin{matrix}a\\a\\a\end{matrix}}\right\} k \\ \left.\vphantom{\begin{matrix}a\\a\\a\end{matrix}}\right\} d-k \end{matrix}$$

III. Haar measure on $\mathcal{U}(d)$ and $\mathcal{SU}(d)$

For an uniformly weighted integration

$$\int_{\mathcal{U}(d)} f(U)dU = \int_{\mathcal{U}(d)} f(U_1 U)dU = \int_{\mathcal{U}(d)} f(UU_2)dU \qquad \forall U_1, U_2 \in \mathcal{U}(d)$$

we need to assign an infinitesimal volume element dU in terms of $\{\lambda_{m,n}\}$

left and right invariant Haar measure

$$dU = d(U_C) = d(U_1 U_C) = d(U_C U_2) \qquad \forall U_1, U_2 \in \mathcal{U}(d)$$

$\rightarrow$ absolute value of the Jacobian determinant

$$J_d = |\det(j_{k,l})| = \left| \det \frac{\partial(u_1, \ldots, u_{d^2})}{\partial(\lambda_{1,1}, \ldots, \lambda_{d,d})} \right| ,$$

$\{u_k\}$ - coefficients of $U_C(\lambda_{1,1}, \ldots, \lambda_{d,d})$ in an orthonormal operator basis

normalized Haar measure

$$dU_d = \frac{J_d}{N_d} \prod_{k,l=1}^{d} d\lambda_{k,l} \qquad N_d \text{ such that } \int_{\mathcal{U}(d)} dU_d = 1 .$$

III. Haar measure on $\mathcal{U}(d)$ and $\mathcal{SU}(d)$

normalized Haar measure on $\mathcal{U}(d)$:

$$dU_d = \frac{1}{N_d} \prod_{m=1}^{d-1} \prod_{n=m+1}^{d} \sin(\lambda_{m,n}) \cos^{2(n-m)-1}(\lambda_{m,n}) \prod_{k,l} d\lambda_{k,l}$$

$$N_d = \frac{(2\pi)^{d(d+1)/2}}{\prod_{m=1}^{d-1} \prod_{n=m+1}^{d} 2(n-m)}$$

normalized Haar measure on $\mathcal{SU}(d)$:

$$dU_d = \frac{1}{N_d} \prod_{m=1}^{d-1} \prod_{n=m+1}^{d} \sin(\lambda_{m,n}) \cos^{2(n-m)-1}(\lambda_{m,n}) \prod_{k,l} d\lambda_{k,l}$$

$$N_d = \frac{2^{d-1} \pi^{d(d+1)/2-1}}{\prod_{m=1}^{d-1} \prod_{n=m+1}^{d} 2(n-m)}$$

Computing group integrals *(explicitly)*

$$\int f(U)dU$$

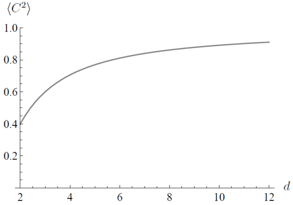
- Many physical problems: $f(U)$ is a polynomial in the components of U.
- Neglecting the computational effort: can be solved analytically (Integral table).
- Non-polynomial functions: use Haar measure dU + numerical methods.

Example 1 - Twirling $\int U \otimes U \rho U^\dagger \otimes U^\dagger dU$

$$\Rightarrow \text{Werner state} \qquad \rho_W = \frac{\mathbb{1} + \beta(\sum_{i,j=1}^{d} |ij\rangle\langle ji|)}{d(d+\beta)}$$

Example 2 - *A priori* entanglement of quantum systems, e.g. $\mathbb{C}^d \otimes \mathbb{C}^d$

$$\overline{E} = \int C^2(|\psi\rangle)d\psi = \frac{(d-1)d}{d^2+1}$$



IV.2 Application: Distillability of quantum states

Distillable quantum states

$$\rho^{\otimes m} \quad \xrightarrow[\textbf{C}\text{lassical } \textbf{C}\text{ommunication}]{\textbf{L}\text{ocal } \textbf{O}\text{perations and}} \quad \left[\tfrac{1}{\sqrt{2}}(|00\rangle + |11\rangle)\right]^{\otimes n}$$

Necessary and sufficient condition for distillability

$\rho^{\otimes m}$ has an entangled $\mathbb{C}^2 \otimes \mathbb{C}^2$ subsystem for finite m

Practical criterion for distillability

States **P**ositive under **P**artial **T**ransposition (PPT) are undistillable **(bound entangled)**

Open question: Does NON-PPT (NPPT) imply distillability?

Conjecture: Werner state $\rho_W = \frac{\mathbb{1}+\beta(\sum_{i,j=1}^{d} |ij\rangle\langle ji|)}{d(d+\beta)}$ NPPT : $-1 \leq \beta < -\frac{1}{d}$

distillable : $-1 \leq \beta < -\frac{1}{2}$

Numerical evidence:

Literature (no parameterization): $d = 3$ $\rho^{\otimes 3} \triangleq 729 \times 729$

Parameterization of $\mathbb{C}^2 \otimes \mathbb{C}^2$ subspaces: $\rho^{\otimes 6} \triangleq 531\,441 \times 531\,441$

Characteristics of the composite parameterization of $\mathcal{U}(d)$

- allows to discard irrelevant phase factors
- parameter ranges are easy to handle
- insightful matrix notation
- computationally beneficial (completely factorized)
- redundancy-free parameterization of
  - orthonormal vectors
  - density matrices
  - subspaces
- leads to a concise formula of the (normalized) Haar measure
- can be used to compute group integrals

THANK YOU

Christoph Spengler, Marcus Huber, Beatrix C. Hiesmayr
A composite parameterization of unitary groups, density matrices and subspaces
J. Phys. A: Math. Theor. 43, 385306 (2010)

Christoph Spengler, Marcus Huber, Beatrix C. Hiesmayr
Composite parameterization and Haar measure for all unitary and special unitary groups
J. Math. Phys. 53, 013501 (2012)

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