JOURNAL OF COMPUTATIONAL PHYSICS 61, 89-104 (1985)

Factorization, Invariant Measure, and Random Selection of Matrices in $SU(n)$ and Other Groups*

GERALD GURALNIK

Los Alamos National Laboratory, Los Alamos, New Mexico 87545

TONY WARNOCK

Cray Research, Inc., Los Alamos, New Mexico 87545

AND

CHARLES ZEMACH

Los Alamos National Laboratory, Los Alamos, New Mexico 87545

Received September 7, 1984; revised December 18, 1984

Matrices of the group $SU(n)$ are parameterized in several ways by a system of generalized polar coordinates. The parameters have an interpretation in terms of a factoring of $SU(n)$ matrices into matrices of $SU(2)$ type. They yield a separable form for the group invariant measure and a continuous map of $SU(n)$ to the unit hypercube in $n^2 - 1$ dimensions such that the invariant measure is the Euclidean measure. Random sampling of $SU(n)$ matrices distributed according to the invariant measure and certain related measures is facilitated. An algorithm for random selection of $SU(2)$ stepping matrices with prescribed trace average and standard deviation is given. Extensions to $U(n)$, $SO(n)$, and $O(n)$ are made.

I. INTRODUCTION

Recent years have seen a major growth in the application and sophistication of Monte Carlo methods for elementary particle physics, and in particular, for lattice gauge formulations of quantum chromodynamics. These methods inevitably strain the memory and computing speed capabilities of the most advanced computers, and strain the budgets of the researchers as well. Such computational physics efforts must seek to optimize the numerical algorithms on which the Monte Carlo methods depend.

* The U.S. Government's right to retain a nonexclusive royalty-free license in and to the copyright covering this paper, for governmental purposes, is acknowledged. The Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36.

0021-9991/85 $3.00

In the applications to quantum chromodynamics, functions of large arrays of $SU(3)$ matrices are averaged with respect to the invariant measure (Haar measure) of $SU(3)$ as a topological group. The Metropolis algorithm [1] for generating such arrays calls for the random selection of "stepping matrices," which are $SU(3)$ matrices distributed with a weighting which biases the selection in favor of a suitably small neighborhood of the unit matrix. Because the "distance" of a matrix from the unit matrix is conveniently expressed in terms of its trace, we can speak of *trace-biased* sampling of matrices.

Strictly speaking, the Metropolis method requires only that the sampling process for stepping matrices be rich enough to move a matrix ergodically through the matrix group in a continuing sequence of steps. We find, however, that the efficiency of the method, and hence the computing speed for thermalization and decorrelation of the $SU(3)$ arrays, is enormously improved with respect to some current approaches by an optimized algorithm for sampling from a distribution which is trace-biased, but otherwise proportional to the invariant measure. The algorithms given here could also be a starting point for sampling more general partially invariant distributions as in the heat-bath technique [2] for lattice gauge calculations.

This is the first of three papers in which we study sampling from invariant or partially invariant distributions of matrices, that is, from matrices distributed over a matrix group uniformly with respect to the invariant measure of the group or distributed in a closely related way. Much of the analysis applies equally well to the matrix groups $SU(n)$ for general n and, with slight modification, to the groups $U(n)$, $O(n)$, and$SO(n)$ as well. The present paper addresses the more general aspects of our method. The second paper focuses on sampling from trace-biased invariant distributions from $SU(3)$. Specific application to generation of lattice configurations for quantum chromodynamics, and the results of numerical experiments on thermalization and decorrelation rates for different lattice sizes and spacings will be given in the third paper.

In the next section, we develop a parameterization of $SU(n)$ matrices in terms of variables derived from the polar coordinate representations of some of the (complex-valued) matrix elements. The scheme follows the polar coordinate decomposition for vectors in a $2n$-dimensional space in a recently described method for sampling of points in or on a hypersphere of arbitrary dimension [3]. These polar parameters have a simple interpretation in terms of parameters for $SU(2)$ matrices which occur as factors in a general factorization scheme for $SU(n)$ matrices. In fact, Section II provides three schemes of factorization and three associated parameterizations. The first is for sampling of $SU(n)$ matrices distributed according to the invariant measure. The third separates out the unitary invariants of the matrix (i.e., the set of eigenvalues) from the set of additionally needed parameters and is more appropriate for trace-biased invariant sampling. The second method is merely a preliminary leading to the third.

Some of our factoring and measure formulas are similar to those of Murnaghan [4]. But the need for a structure to facilitate efficient random sampling motivated significant departures from Murnaghan's treatment, as well as extensions of it. Section III develops formulas for invariant measure in terms of various parameterizations. Section IV gives an algorithm for trace-biased, but otherwise invariant, sampling of $SU(2)$ matrices in which the average and the standard deviation of the trace distribution are independent input parameters. Section V outlines briefly how the same techniques apply to parameterization, factoring, invariant measure, and sampling of $SO(n)$. Extension to $U(n)$ and $O(n)$ is also noted.

II. Parameterizations for $SU(n)$ Matrices

1. *A Factorization Formula*

Let A_{ij} be the matrix elements of an $SU(n)$ matrix, i.e., an $n \times n$ unitary unimodular matrix A. Let A act on an n-dimensional vector space W_n, where W_n is represented as a direct sum,

$$W_n = V^{(1)} \oplus V^{(2)} \oplus \cdots \oplus V^{(N)},$$

of 1-dimensional vector spaces $V^{(i)}$. We represent the rows of A as vectors:

$$\mathbf{A}_i = \{A_{i1}, A_{i2}, \dots, A_{in}\}.$$

The general $n \times n$ complex matrix is specified by $2n^2$ real parameters, but the orthonormality and phase conditions on A:

$$\mathbf{A}_i^* \cdot \mathbf{A}_j = \delta_{ij}, \qquad 1 \leqslant i \leqslant j \leqslant n, \tag{2.1}$$

$$\det A = +1, \tag{2.2}$$

impose $n^2 + 1$ constraints, leaving $n^2 - 1$ free parameters.

We now provide a set of generalized polar coordinates adequate to parameterize such $SU(n)$ matrices for arbitrary n. This will, at the same time, yield a prescription for factoring $SU(n)$ matrices into matrices of $SU(2)$ type.

To begin, let the last row of A be expressed in terms of $2n$ polar parameters as follows:

$$\begin{aligned}
A_{n1} &= \rho_{n1} \exp(i\phi_{n1}) \\
A_{n2} &= \bar{\rho}_{n1} \rho_{n2} \exp(i\phi_{n2}) \\
&\vdots \\
A_{ni} &= \bar{\rho}_{n1} \bar{\rho}_{n2} \cdots \bar{\rho}_{n,i-1} \rho_{ni} \exp(i\phi_{ni}) \\
&\vdots \\
A_{nn} &= \bar{\rho}_{n1} \bar{\rho}_{n2} \cdots \bar{\rho}_{n,n-1} \rho_{nn} \exp(i\phi_{nn}).
\end{aligned} \tag{2.3}$$

The phases ϕ_{ni} lie on the interval $(0, 2\pi)$ and the radial parameters ρ_{ni} are on $(0, 1)$. The complementary radial parameters $\bar{\rho}_{ni}$ are also on $(0, 1)$ and are related to the ρ_{ni} by

$$(\rho_{ni})^2 + (\bar{\rho}_{ni})^2 = 1.$$

These conditions can be met whenever $|\mathbf{A}_n|^2 \leqslant 1$. In fact,

$$1 - |\mathbf{A}_n|^2 = \prod_{i=1}^{n} (\bar{\rho}_{ni})^2, \tag{2.4}$$

so that when the normalization condition is applied to $\mathbf{A}_n$, then ρ_{nn} is no longer a variable; instead $\rho_{nn} = 1$, $\bar{\rho}_{nn} = 0$.

Let $(n-1, n)$ denote the $SU(n)$ matrix which acts as the SU_2 matrix

$$\begin{pmatrix} \bar{\rho}_{n,n-1} \exp(-i\phi_{nn}) & -\rho_{n,n-1} \exp(-i\phi_{n,n-1}) \\ \rho_{n,n-1} \exp(i\phi_{n,n-1}) & \bar{\rho}_{n,n-1} \exp(i\phi_{n,n}) \end{pmatrix}$$

on the subspace $V^{(n-1)} \oplus V^{(n)}$ of W_N and which acts as the unit matrix on the complement of this subspace. And for $1 \leqslant i \leqslant n-2$, let $(\overline{i, n})$ denote the $SU(n)$ matrix which acts on $V^{(i)} \oplus V^{(n)}$ as

$$\begin{pmatrix} \bar{\rho}_{ni} & -\rho_{ni} \exp(-i\phi_{ni}) \\ \rho_{ni} \exp(i\phi_{ni}) & \bar{\rho}_{ni} \end{pmatrix}$$

and as the unit matrix on the complement subspace. The $(\overline{i, n})$ matrices will be referred to as "reduced" matrices. Their SU_2 parts have real diagonal elements and, in the usual map from SU_2 to SO_3, correspond to 3-dimensional rotations whose axes of rotation lie in the xy plane.

Next define an $SU(n)$ matrix P_n by

$$P_n = (\overline{1, n})(\overline{2, n}) \cdots (\overline{n-2, n})(n-1, n). \tag{2.5}$$

The matrix elements of P_n can be written out according to a systematic rule obtained by induction on the product (2.5) and detailed in Subsection 4, below.

The essential feature of this construction is that the last row of P_n *coincides* with the last row of A. Now consider the last column of AP_n^{-1}:

$$(AP_n^{-1})_{\text{in}} = A_{ij}(P_n)^*_{nj} = A_{ij} \cdot A^*_{nj} = \delta_{in}.$$

For the last now, we have

$$(AP_n^{-1})_{ni} = A_{nj}(P_n)^*_{ij} = P_{nj}(P_n)^*_{ij} = \delta_{ni}.$$

Thus, we can write

$$AP_n^{-1} = \begin{pmatrix} B & 0 \\ 0 & 1 \end{pmatrix}, \tag{2.6a}$$

and

$$A = \begin{pmatrix} B & 0 \\ 0 & 1 \end{pmatrix} P_n, \tag{2.6b}$$

where B is an $SU(n-1)$ matrix. This is the first step in the factorization of A into matrices of SU_2-type. The elements B_{ij} are functions of the polar coordinates already defined and of the elements A_{ij} for $i, j \leqslant n-1$. Useful expressions for these B_{ij} are given below in Subsection 4. Then the last row of B can be used to define a new set of polar parameters $\rho_{n-1,i}$, $\phi_{n-1,i}$, and an $SU(n-1)$ matrix P_{n-1} and so on. The final factorized form is

$$A = P_2 P_3 \cdots P_n. \tag{2.7}$$

This product depends on $\frac{1}{2}(n^2+n-2)$ phase parameters ϕ_{ij}, $2 \leqslant i \leqslant n$, $1 \leqslant j \leqslant 1$, and $\frac{1}{2}(n^2-n)$ radial parameters ρ_{ij}, $1 \leqslant j < i \leqslant n$, for a total of n^2-1 parameters, as is appropriate for $SU(n)$.

For the case $n=2$, we have, in this notation

$$A = (12) = \begin{pmatrix} \bar{\rho}_{21} \exp(-i\phi_{22}) & -\rho_{21} \exp(-i\phi_{21}) \\ \rho_{21} \exp(i\phi_{21}) & \bar{\rho}_{21} \exp(i\phi_{22}) \end{pmatrix}. \tag{2.8}$$

For the case $n=3$, we have

$$\begin{aligned} A = {} & (12)(\overline{13})(23) \\ = {} & \begin{pmatrix} \bar{\rho}_{21}\bar{\rho}_{31} \exp(-i\phi_{22}) & A_{12} & A_{13} \\ \rho_{21}\bar{\rho}_{31} \exp(i\phi_{21}) & A_{22} & A_{23} \\ \rho_{31} \exp(i\phi_{31}) & \bar{\rho}_{31}\rho_{32} \exp(i\phi_{32}) & \bar{\rho}_{31}\bar{\rho}_{32} \exp(i\phi_{33}) \end{pmatrix} \end{aligned} \tag{2.9}$$

with

$$\begin{aligned} A_{12} &= -\rho_{21}\bar{\rho}_{32} \exp[i(-\phi_{21}-\phi_{33})] - \bar{\rho}_{21}\rho_{31}\rho_{32} \exp[i(-\phi_{22}-\phi_{31}+\phi_{32})] \\ A_{22} &= \bar{\rho}_{21}\bar{\rho}_{32} \exp[i(\phi_{22}-\phi_{33})] - \rho_{21}\rho_{31}\rho_{32} \exp[i(\phi_{21}-\phi_{31}+\phi_{32})] \\ A_{13} &= \rho_{21}\rho_{32} \exp[i(-\phi_{21}-\phi_{32})] - \bar{\rho}_{21}\rho_{31}\bar{\rho}_{32} \exp[i(-\phi_{22}-\phi_{31}+\phi_{33})] \\ A_{23} &= -\bar{\rho}_{21}\rho_{32} \exp[i(\phi_{22}-\phi_{32})] - \rho_{21}\rho_{31}\bar{\rho}_{32} \exp[i(\phi_{21}-\phi_{31}+\phi_{33})]. \end{aligned}$$

In the SU_3 case, there are three radial parameters and five phase parameters. When A is given, the parameters are fixed by the phases of A_{11}, A_{21}, A_{31}, A_{32}, A_{33} and the magnitudes of A_{31}, A_{21}, and A_{32}. Or, if the parameters are given, e.g., by a Monte Carlo sampling, the above formulas give the elements of A.

2. *A Second Factoring*

Let a new set of phases be defined by $\alpha_n = \phi_{nn}$ and $\psi_{ni} = \phi_{ni} - \phi_{nn}$ for $1 \leqslant i \leqslant n-1$. As an alternative to Eq. (2.5), set

$$P'_n = (\overline{1,n})' \, (\overline{2,n})' \cdots (\overline{n-2,n})' \, (\overline{n-1,n})' \tag{2.10}$$

where $(\overline{i,n})'$ is an $SU(n)$ matrix which acts on $V^{(i)} \oplus V^{(n)}$ like the reduced SU_2 matrix

$$\begin{pmatrix} \bar{\rho}_{ni} & -\rho_{ni}\exp(-i\psi_{ni}) \\ \rho_{ni}\exp(i\psi_{ni}) & \bar{\rho}_{ni} \end{pmatrix}$$

and acts like the unit matrix on the complement space. Then the relation between the last rows of A and P'_n is

$$A_{ni} = \exp(i\alpha_n)(P'_n)_{ni}, \qquad 1 \leqslant i \leqslant n,$$

and the analog of Eq. (2.6b) is

$$A = \begin{pmatrix} B' & 0 \\ 0 & \exp(i\alpha_n) \end{pmatrix} P'_n, \tag{2.11}$$

where B' is $SU(n-1)$. This process can be iterated as before to yield a complete factorization

$$A = d(\boldsymbol{\alpha})\, P'_2 P'_3 \cdots P'_n. \tag{2.12}$$

Here $d(\boldsymbol{\alpha})$ is a diagonal $SU(n)$ matrix with diagonal elements $\exp(i\alpha_i)$. The phase α_1, which is the last to be defined in this process, is not independent of the other α-phases because the α_i sum to zero. This parameterizes A in terms of $\frac{1}{2}(n^2-n)$ ρ variables, identical to the ρs of the previous section, an equal number of ψ variables, and $n-1$ independent α variables. The relation between the old and new phases is

$$\begin{aligned} &\alpha_n = \phi_{nn}, \\ &\alpha_i = \phi_{ii} - \phi_{i+1,i+1} \qquad \text{for} \qquad 2 \leqslant i \leqslant n-1, \\ &\alpha_1 = -\phi_{22}, \end{aligned} \tag{2.13a}$$

and

$$\begin{aligned} &\psi_{nj} = \phi_{nj} - \phi_{nn} \qquad \text{for} \qquad 1 \leqslant j \leqslant n-1, \\ &\psi_{ij} = \phi_{ij} - \phi_{ii} + \phi_{i+1,i+1} \qquad \text{for} \qquad 1 \leqslant j < i \leqslant n-1. \end{aligned} \tag{2.13b}$$

The parameterization defined by Eq. (2.7) is our candidate for the efficient random generation of $SU(n)$ matrices distributed according to the invariant measure of the group. If, however, the random selection of matrices is to be biased with respect to one or more unitary invariants of the matrices, such as the set of eigenvalues, or the trace, an alternative representation is needed. The second representation, Eq. (2.12), is introduced as a step toward this alternative.

3. *A Third Factoring*

Given an $SU(n)$ matrix A, let $D(\boldsymbol{\theta})$ be the diagonal matrix whose diagonal elements are its eigenvalues $\exp(i\theta_i)$, $1 \leqslant n$, taken in any order. Let U be an $SU(n)$ matrix which diagonalizes A as follows:

$$A = U^{-1} D(\boldsymbol{\theta})\, U. \tag{2.14}$$

The eigenphases are constrained by $\sum \theta_i = 0 \pmod{2\pi}$. Eq. (2.14) does not specify U uniquely. If X is any diagonal $SU(n)$ matrix, XU will do as well because X commutes with $D(\boldsymbol{\theta})$. One way to pick a unique member of the class of $\{XU\}$ is via the representation (2.12): Select the V in this class whose $D(\boldsymbol{\alpha})$ factor is unity. Thus our third factorization has the form

$$A = V(\boldsymbol{\rho}, \boldsymbol{\psi})^{-1}\, D(\boldsymbol{\theta})\, V(\boldsymbol{\rho}, \boldsymbol{\psi}) \tag{2.15}$$

where

$$V(\boldsymbol{\rho}, \boldsymbol{\psi}) = P'_2 P'_3 \cdots P'_n.$$

Then $V(\boldsymbol{\rho}, \boldsymbol{\psi})$ depends on $\frac{1}{2}(n^2 - n)$ radial variables and an equal number of phase variables as prescribed by (2.10), and $D(\boldsymbol{\theta})$ depends on $n-1$ eigenphases. Again, A depends on $n^2 - 1$ variables.

4. *Additional Details*

First, let

$$q_i(n) = \prod_{k=1}^{i} \bar{\rho}_{nk} \qquad \text{for } 1 \leqslant i \leqslant n-1, \tag{2.16}$$

and let $q_0(n) = 1$. Then the matrix elements of P_n, Eq. (2.5), can be summarized compactly as follows:

$$\begin{aligned}
(P_n)_{nj} &= \exp(i\phi_{nj})\, \rho_{nj} q_{j-1}(n) = A_{nj} && \text{for} \quad 1 \leqslant j \leqslant n,\\
(P_n)_{ij} &= 0 && \text{for} \quad 1 \leqslant j < i < n,\\
(P_n)_{n-1,n-1} &= \exp(-i\phi_{nn})\, \bar{\rho}_{n,n-1}, && (P_n)_{ii} = \bar{\rho}_{ni} \text{ for } 1 \leqslant i \leqslant n-2,\\
(P_n)_{ij} &= -\exp[i(-\phi_{ni} + \phi_{nj})]\, \rho_{ni}\rho_{nj} q_{j-1}(n)/q_i(n)\\
&= -\exp(-i\phi_{ni})\, \rho_{ni} A_{nj}/q_i(n), && 1 \leqslant i \leqslant n-2,\ i < j \leqslant n,\\
(P_n)_{n-1,n} &= -\exp(-i\phi_{n,n-1})\, \rho_{n,n-1}\\
&= -\exp[-i(\phi_{n,n-1} + \phi_{nn})]\, \rho_{n,n-1} A_{nn}/q_{n-1}(n).
\end{aligned}$$

Second, from this specification and (2.6a), we can express the components of B as

$$B_{ij} = A_{ij}\bar{\rho}_{nj} + \left(\sum_{k=1}^{j} A^*_{nk} A_{ik}\right) \exp(i\phi_{nj})\, \rho_{nj}/q_j(n), \qquad 1 \leqslant j \leqslant n-2,$$

$$B_{i,n-1} = \Bigg[A_{i,n-1}\bar{\rho}_{n-1,n-1} + \left(\sum_{k=1}^{n-1} A^*_{nk} A_{ik}\right) \exp(i\phi_{n,n-1})\, \rho_{n,n-1}/q_{n-1}(n)\Bigg] \exp(i\phi_{nn}),$$

for all $i \leqslant n-1$. To obtain the elements of B on and below the principal diagonal from this formula, it is sufficient to know the elements of A on and below the principal diagonal. Then, calculation of the complete factorization Eq. (2.7) and of the polar parameters from a given A utilizes only the elements of A on and below the principal diagonal.

III. Invariant Measure for $SU(n)$

1. *The Measure in Terms of Polar Coordinates*

We adopt a complex notation for differentials and for δ-functions. For example,

$$d^{2n}\mathbf{A}_i = \prod_{j=1}^{n} (d\,\mathrm{Re}\, A_{ij})(d\,\mathrm{Im}\, A_{ij}),$$

$$\delta^{(2)}(\mathbf{A}_i^* \cdot \mathbf{A}_j) = \delta(\mathrm{Re}\, \mathbf{A}_i^* \cdot \mathbf{A}_j)\, \delta(\mathrm{Im}\, \mathbf{A}_i^* \cdot \mathbf{A}_j).$$

If M is a complex matrix, then $A = A'M$ defines a linear transformation on the rows of A and

$$d^{2n}\mathbf{A}_i = |\det M|^2\, d^{2n}\mathbf{A}'_i.$$

The invariant measure $\mu_n(A)$ on $SU(n)$ can be expressed formally by

$$\mu_n(A) \cong ⨍ \Delta_n(A)\, \delta(\mathrm{phase}(\det A)) \prod_{i=1}^{n} d^{2n}\mathbf{A}_i. \tag{3.1}$$

The sign $\cong$ means the two sides differ at most by a constant factor. Here, $\Delta_n(A)$ is the product of n δ-functions of type $\delta(1 - |\mathbf{A}_i|^2)$ for row normalization and $\frac{1}{2}n(n-1)$ δ-functions of type $\delta^{(2)}(\mathbf{A}_i^* \cdot \mathbf{A}_j)$ for row orthogonality. Because orthonormality implies $|\det A| = 1$, only phase $(\det A)$ must be set as an additional condition. The A_{ij} comprise $2n^2$ real variables initially varying on $(-\infty, \infty)$. The crossed integral sign calls for enough integrations to absorb the δ-functions. To verify right (and hence left) invariance of this measure, one notes that right translation of A by a group element defines a unitary, unimodular transformation on each row, leaving $\det A$, the orthonormality relations, and $d^{2n}\mathbf{A}_i$ invariant.

For the case $n=2$, integration of (3.1) over $d^{(4)}\mathbf{A}_1$ yields

$$d\mu_2(A) \cong \int \delta(1-|\mathbf{A}_2|^2)\, d^4\mathbf{A}_2,$$

displaying the SU_2 invariant measure as equivalent to the surface measure ds_4 for a hypersphere in 4-space (as is well known). The Euclidean coordinates of the 4-space are here represented by the two real and two imaginary components of the last row of A.

More generally, $d\mu_n$ can be related to $d\mu_{n-1}$ as follows: Set $d\mu_n(A) = \sigma d\beta ds_{2n}$, where

$$\sigma \cong \int \prod_{i=1}^{n-1} \delta^{(2)}(\mathbf{A}_n^* \cdot \mathbf{A}_i)\, d^2A_{in} = |A_{nn}|^{-(2n-2)},$$

$$d\beta \cong \int \Delta_{n-1}(A)\, \delta(\text{phase}(\det A)) \prod_{i,j=1}^{n-1} d^2A_{ij},$$

$$ds_{2n} \cong \int \delta(1-|\mathbf{A}_n|^2)\, d^{2n}\mathbf{A}_n.$$

Here, $\Delta_{n-1}(A)$ is the product of δ-functions for orthonormality of the first $n-1$ rows of A. In the $2n$-space spanned by the real and imaginary elements of the last row of A, ds_{2n} is the surface measure of the unit hypersphere.

Now let P_n be any $SU(n)$ matrix whose last row coincides with the last row of A. Let $\hat{A}$ and $\hat{P}$ be $(n-1)\times(n-1)$ matrices formed from A and P_n by deleting the last rows and last columns. Then, the relations

$$A = \begin{pmatrix} B & 0 \\ 0 & 1 \end{pmatrix} P_n, \qquad \hat{A} = B\hat{P}_n$$

define a transformation between $(n-1)^2$ variables A_{ij}, $1 \leqslant i, j \leqslant n-1$, and $(n-1)^2$ new variables B_{ij} comprising the matrix B. The first relation gives A as a right translation by the $SU(n)$ matrix P_n, hence

$$\Delta_{n-1}(A) = \Delta_{n-1}(B) \qquad \text{and} \qquad \det A = \det B.$$

The second relation is the specific transformation, row by row, of B to A, so that for $1 \leqslant i \leqslant n-1$,

$$\prod_{j=1}^{n-1} d^2A_{ij} = |\det \hat{P}_n|^2\, d^{2n-2}\mathbf{B}_i.$$

Hence,

$$d\beta \cong d\mu_{n-1}(B) |\det \hat{P}_n|^{2n-2}.$$

Moreover,

$$A^*_{nn} = (P_n)^*_{nn} = (P_n^{-1})_{nn} = [\text{cofactor of } (P_n)_{nn}]/\det P_n = \det \hat{P}_n.$$

Then, σ cancels against the det factor in $d\beta$ and

$$d\mu_n(A) \cong d\mu_{n-1}(B)\, ds_{2n}.$$

This process can be continued by defining a series of P_k and ds_{2k} down to $k=2$, giving

$$d\mu_n(A) = \prod_{k=2}^{n} ds_{2k}. \tag{3.2}$$

Finally, we make this formalism concrete by introducing the generalized polar coordinates to parameterize the P_k and hence A. Then (compare with (2.4) and (2.16))

$$\begin{aligned} ds_{2k} &\cong \int \delta([q_k(k)]^2) \prod_{j=1}^{k} [q_{j-1}(k)]^2\, d(\bar{\rho}_{kj})^2\, d\phi_{kj} \\ &\cong d\phi_{kk} \prod_{j=1}^{k-1} d(\bar{\rho}_{kj})^{2k-2j}\, d\phi_{kj}. \end{aligned}$$

The complete representation of the invariant measure in terms of the polar parameters is then

$$d\mu_n(A) \cong d\mu_n(\boldsymbol{\rho}, \boldsymbol{\phi}) = \prod_{i=2}^{n} d\phi_{ii} \prod_{j=1}^{i-1} d(\bar{\rho}_{ij})^{2i-2j}\, d\phi_{ij}. \tag{3.3}$$

For $n=2$ and $n=3$, this reads

$$d\mu_2(A) \cong d\mu_2(\boldsymbol{\rho}, \boldsymbol{\phi}) = d(\bar{\rho}_{21})^2\, d\phi_{21}\, d\phi_{22}, \tag{3.4}$$

$$d\mu_3(A) \cong d\mu_3(\boldsymbol{\rho}, \boldsymbol{\phi}) = d(\bar{\rho}_{21})^2\, d(\bar{\rho}_{31})^4\, d(\bar{\rho}_{32})^2\, d\phi_{21}\, d\phi_{22}\, d\phi_{31}\, d\phi_{32}\, d\phi_{33}. \tag{3.5}$$

If we desire an invariant measure normalized to

$$\int d\mu_n(A) = 1,$$

we have only to replace each ϕ_{ij} by $(2\pi)^{-1}\, \phi_{ij}$.

The formula (3.3) for invaiant measure is completely separable with respect to the polar parameters. When the quantities $(\bar{\rho}_{ij})^{2i-2j}$ and $(2\pi)^{-1}\, \phi_{ij}$ are taken as the group parameters, we have a continuous map from the group $SU(n)$ to the unit hypercube in $n^2 - 1$ dimensions such that the invariant measure on the hypercube is the Euclidean measure. Preservation of the topology requires that for each i, j, the end-point values $\phi_{ij} = 0$ and $\phi_{ij} = 2\pi$ are identified with the same group element, and additional identifications are implied when ρ_{ij} or $\bar{\rho}_{ij}$ vanish.

2. *The Sampling Process*

To generate $SU(n)$ matrices distributed according to $d\mu_n$, one would first generate the polar parameters $\bar{\rho}_{ij}$, ϕ_{ij} according to Eq. (3.3), then compute the ρ_{ij} and the P_k, and calculate A from (2.7). To generate a set of $\bar{\rho}$ distributed according to $d(\bar{\rho})^m$, set either

$$\bar{\rho} = \mathrm{Max}(u_1, u_2, ..., u_m)$$

or

$$\bar{\rho} = (u)^{1/m},$$

where the us are uniformally distributed random numbers on (0, 1). There will be an m_0 such that the first way is faster for $m \leqslant m_0$ and slower for $m > m_0$. In our experiments, $m_0 \approx 7$ for a Cray in scalar mode, and $m_0 \approx 5$ for a Cray in vector mode. For large n, computer time goes like n^4.

This may be compared with the well-known method which begins by uniform sampling (n times) of the surface of a unit hypersphere in $2n$ dimensions. The samples become the rows of an $n \times n$ complex matrix which is converted to an $SU(n)$ matrix by Gram–Schmidt orthonormalization. For large n, computer time is proportional to n^3.

Therefore, our polar coordinate method will not be competitive in computing speed with the conventional method in the limit of large n. But it appears to be faster for not-too-large n values, the exact range depending on the choice of computer, choice of compiler, and the way the algorithm is embedded in the intended application. As an example, we found the present method 58% faster than the Gram–Schmidt process when both were programmed for $SU(3)$ sampling on the Cray 1-S and Cray XMP in vector mode.

3. *Invariant Measure for the Factoring* $A = V^{-1}DV$

The ψ and α angles of the second factoring are simple translations of the ϕs. The measure in terms of the parameters of the second factoring can be expressed as

$$d\mu_n(A) \cong dv_n(\rho, \psi)\, dv'_n(\alpha), \tag{3.7}$$

where

$$dv_n(\boldsymbol{\rho}, \boldsymbol{\psi}) = \prod_{i=2}^{n} \prod_{j=1}^{i-1} d(\bar{\rho}_{ij})^{2i-2j}\, d\psi_{ij} \tag{3.8a}$$

and

$$dv'_n(\boldsymbol{\alpha}) = \prod_{i=2}^{n} d\alpha_i. \tag{3.8b}$$

Now consider an ensemble of matrices A defined by

$$A = U_1^{-1} U_2 U_1,$$

where the U_1 and U_2 matrices are both distributed according to the $SU(n)$ measure. Then A is distributed according to $d\mu_n(A)$ because the A-ensemble differs from the U_2-ensemble only by left and right translations. Let $U_2 = U_3^{-1} D(\boldsymbol{\theta})\, U_3$, where U_3 is $SU(n)$ and $D(\boldsymbol{\theta})$ is a diagonal form of U_2. Then $D(\boldsymbol{\theta})$ is also a diagonal form of A, with eigenvalues $\exp(i\theta_i)$ taken in any order. The measure for U_2 can be expressed as a product (see [4], Chap. 8]) $d\lambda_n(\boldsymbol{\theta})\; d\lambda'_n(U_3)$ of measures depending on $D(\boldsymbol{\theta})$ and U_3 separately. In particular,

$$\begin{aligned} d\lambda_n(\boldsymbol{\theta}) &= \prod_{i<j} \left| \frac{1}{2} [\exp(i\theta_i) - \exp(i\theta_j)] \right|^2 \prod_{k=2}^{n} d\theta_k \\ &= \prod_{i<j} \sin^2 \frac{\theta_i - \theta_j}{2} \prod_{k=2}^{n} d\theta_k. \end{aligned} \tag{3.9}$$

The matrices $U_4 = U_3 U_1$ are also invariantly distributed, being left translations of U_1. Let $U_4 = d(\alpha)\, V(\boldsymbol{\rho}, \boldsymbol{\psi})$ be the factoring of U_4 according to the second rule, Eq. (2.12), with $d(\alpha)$ diagonal. Then we arrive at the representations

$$A = V^{-1}(\boldsymbol{\rho}, \boldsymbol{\psi})\, D(\theta)\, V(\boldsymbol{\rho}, \boldsymbol{\psi}) \tag{3.10}$$

and

$$d\mu_n(A) \cong dv_n(\boldsymbol{\rho}, \boldsymbol{\psi})\, d\lambda_n(\boldsymbol{\theta}) \tag{3.11}$$

with dv_n, $d\lambda_n$ given by (3.8a) and (3.9). This provides an explicit separation, both in the parametric representation of an $SU(n)$ matrix, and in the representation of the invariant measure, of the $n-1$ parameters θ_i which determine the unitary invariants of A.

IV. An Elementary Example: Trace-Biased Sampling for $SU(2)$

For $A = V^{-1} D V$ in the SU_2 case, we have, dropping the unnecessary subscripts,

$$\begin{aligned} D(\theta) &= \begin{pmatrix} \exp(-i\theta) & 0 \\ 0 & \exp(i\theta) \end{pmatrix}, \\ A &= \begin{pmatrix} \cos\theta - i(2\bar{\rho}^2 - 1)\sin\theta & 2i\rho\bar{\rho}\exp(-i\phi)\sin\theta \\ 2i\rho\bar{\rho}\exp(i\phi)\sin\theta & \cos\theta + i(2\bar{\rho}^2 - 1)\sin\theta \end{pmatrix}, \end{aligned} \tag{4.1}$$

and

$$d\mu_2(a) \cong \sin^2\theta\, d\theta\, d(\bar{\rho})^2\, d\phi. \tag{4.2}$$

The matrix A is in the neighborhood of the unit matrix I when θ is close to 0, that is, when $t = \text{trace } A = 2\cos\theta$ is close to 2. To sample stepping matrices for an $SU(2)$ lattice calculation, i.e., matrices biased toward I but otherwise uniformly distributed in $SU(2)$ measure, one may select $\bar{\rho}$, ϕ according to $d(\bar{\rho})^2\, d\phi$ and θ (or t) according to

$$d\lambda = f(\cos\theta)\sin^2\theta\, d\theta \equiv dF(t),$$

where $f(\cos\theta)$, or equivalently $F(t)$, defines a weighted distribution, and depends on parameters to be tuned by numerial experiments or physical insight to maximize thermalization and decorrelation rates in lattice generation. If $d\lambda$ does not go like $\theta^2\, d\theta$ near $\theta = 0$, i.e., like $(2-t)^{1/2}\, dt$ near $t = 2$, oversampling of stepping matrices near I may occur, leading to calculational inefficiency.

Our objective can be formulated as follows: Define a t distribution which can be easily sampled, is properly behaved near $t = 2$, and whose average $\bar{t}$ and standard deviation σ can be prescribed over a useful working range including, say, the range $1 \leqslant \bar{t} \leqslant 2$.

To implement this, let r and s be randomly selected from the uniform distribution on (0, 1), let b and w be real positive parameters, to be determined from $\bar{t}$ and σ as specified below, and let t be determined by solving

$$s = \exp\{-[(2-t)/(b+wr)]^{3/2}\}. \tag{4.3}$$

Then t can be between $-\infty$ and 2, but in practice, t values less than -2, which cannot represent the trace of an $SU(2)$ matrix, will occur infrequently and can be dropped or reset to $t = -2$. The effective t-distribution is then $dF(t)$, where

$$F(t) = \int_{r=0}^{1} \exp\{-[(2-t)/(b+wr)]^{3/2}\}\, dr.$$

Then $\int dF(t) = 1$ and dF/dt goes like $(2-t)^{1/2}$ for t near 2.

We identify certain Γ-function integrals

$$c_1 = \int_{\infty}^{0} z\, d[\exp(-z^{3/2})] = \Gamma(\tfrac{5}{3}) = 0.90274\,52930$$

and

$$c_2 = \int_{\infty}^{0} z^2 d[\exp(-z^{3/2})] = \Gamma(\tfrac{7}{3}) = 1.19063\,93488.$$

Then

$$\bar{t} = \int t dF(t) = 2 - c_1(b + \tfrac{1}{2}w)$$

$$\sigma^2 = \int (t^2 - (\bar{t})^2)\, dF(t) = \frac{c_2 - c_1^2}{c_1^2}(2-\bar{t})^2 + w^2/12.$$

Hence,

$$w^2 = 12[c_1^2\sigma^2 - (c_2 - c_1^2)(2-\bar{t})^2]/c_1^2 c_2, \qquad b = (2-\bar{t})/c_1 - \tfrac{1}{2}w.$$

The sampling algorithm for the trace-biased distribution is then: calculate b and w from prescribed values of $\bar{t}$ and σ; choose r and s randomly on $(0, 1)$; and solve (4.3) for t. Then sample $\bar{\rho}$ and ϕ from (4.2) and compute A from (4.1).

V. Parameterization and Invariant Measure for $SO(n)$

1. *The Analogy to* $SU(n)$

We develop here two alternative parametrizations of $SO(n)$ which parallel the work of Section III. The first provides a factoring of an $SO(n)$ matrix into a product of matrices of $SO(2)$ type, but the form taken on by the invariant measures makes random selection of the parameters inconvenient and perhaps unfeasible for practical application for n larger than three or four. The parameters and factored forms are substantially those of Murnaghan [4] for $SO(n)$. The second parameterization is a variant that does allow efficient sampling, but apparently loses the connection to an elegant factorization.

If A is an $SO(n)$ matrix, Eq. (3.1) still defines the invariant measure provided the A_{ij} are understood to be real and δ (phase(det A)) is deleted. A restriction to $\det A = 1$ must be added. Let P_n be redefined as an $SO(n)$ matrix whose last row coincides with the last row of A, and let B be the associated $SO(n-1)$ matrix in analogy to Eq. (2.6). P_n is not tied to any specific parametrization at this point. The development follows that of Section III in form, if not in all detail, and the analog of (3.2) is

$$d\mu_n(A) = \prod_{k=2}^{n} ds_k, \tag{5.1}$$

with

$$A = P_2 P_3 \cdots P_n$$

and ds_k being the surface element for a hypersphere in a k-dimensional space whose Euclidean coordinates are the k (real) elements of the last row of P_k.

2. *First Parametrization*

Suppose we take over the parametrization of Eq. (2.3), but replace the phase factors by unity. We must allow both ρ_{ij} and $\bar{\rho}_{ij}$ to vary on $(-1, +1)$ and allow both signs in $\rho_{ij} = \pm(1-(\bar{\rho}_{ij})^2)^{1/2}$ (with equal probability in a sampling calculation). One can also set $\rho_{ij} = \cos\gamma_{ij}$, $\bar{\rho}_{ij} = \sin\gamma_{ij}$, and allow γ_{ij} to vary on $(0, 2\pi)$.

Then we can define $(\overline{ij})$ as an $SO(n)$ matrix of $SO(2)$ type on $V^{(i)} \oplus V^{(j)}$, $i<j$, whose $SO(2)$ part is

$$\begin{pmatrix} \bar{\rho}_{ij} & -\rho_{ij} \\ \rho_{ij} & \bar{\rho}_{ij} \end{pmatrix}.$$

The factorization of A is expressed by

$$A = \prod_{k=2}^{n} P_k$$

where

$$P_k = (1\tilde{k})(2\tilde{k}) \cdots (k-1, \tilde{k}). \tag{5.2}$$

There are $\frac{1}{2}n(n-1)\,\rho$ parameters, as is appropriate for $SO(n)$. The invariant measure is given by (5.1) with

$$ds_k = \prod_{i=1}^{k-1} (\bar{\rho}_{ki})^{k-i-2}\, d\rho_{ki} = \prod_{i=1}^{k-1} (\sin \gamma_{ki})^{k-i-1}\, d\gamma_{ki}.$$

The sampling difficulty referred to above is that for $n \geqslant 4$, there will be distributions like $(\bar{\rho})^{m-1}\, d\rho$ or $(\sin \gamma)^m\, d\gamma$ with $m \geqslant 2$, which cannot be sampled as straightforwardly as $d(\bar{\rho})^{2m}$ which occurred in the $SU(n)$ context.

3. *Second Parametrization*

The simplicity of the task of randomly selecting the parameters can be recovered, at the cost of losing the factorings (5.2) for the P_k, as follows:

If $k = 2m =$ even, let $x_i = (P_k)_{ki}$, $1 \leqslant i \leqslant k$, be the elements of the last row of P_k, and parametrize as follows:

$$\begin{aligned}
x_1 &= \rho_{k1} \cos \theta_{k1}, & x_2 &= \rho_{k1} \sin \theta_{k1},\\
x_3 &= \bar{\rho}_{k1} \rho_{k2} \cos \theta_{k2}, & x_4 &= \bar{\rho}_{k1} \rho_{k2} \sin \theta_{k2},\\
&\vdots & &\\
x_{2i-1} &= \bar{\rho}_{k1} \bar{\rho}_{k2} \cdots \bar{\rho}_{k,i-1} \rho_{ki} \cos \theta_{ki}, & x_{2i} &= \bar{\rho}_{k1} \bar{\rho}_{k2} \cdots \bar{\rho}_{k,i-1} \rho_{ki} \sin \theta_{ki},\\
&\vdots & &\\
x_{2m-1} &= \bar{\rho}_{k1} \bar{\rho}_{k2} \cdots \bar{\rho}_{k,m-1} \rho_{km} \cos \theta_{kn}, & x_{2m} &= \bar{\rho}_{k1} \bar{\rho}_{k2} \cdots \bar{\rho}_{k,n-1} \rho_{km} \sin \theta_{km}.
\end{aligned}$$

Then we find a direct analogy to the m-dimensional complex case:

$$ds_k \cong d\theta_{km} \prod_{j=1}^{m-1} d(\bar{\rho}_{kj})^{k-2j}\, d\theta_{kj} \qquad (\text{with } \rho_{km} = 1). \tag{5.3}$$

And if $k = 2m+1$, there is one additional transformation,

$$x_{2m+1} = \bar{\rho}_{k1} \bar{\rho}_{k2} \cdots \bar{\rho}_{km} \rho_{k,m+1}$$

and

$$ds_k \cong \prod_{j=1}^{m} d(\bar{\rho}_{kj})^{k-2j}\, d\theta_{kj} \qquad (\text{with } \rho_{k,m+1} = \pm 1). \tag{5.4}$$

Let an $n \times n$ matrix be formed with $x_1, x_2, \ldots, x_n$ as the last row and let the kth row, for $1 \leqslant k \leqslant n-1$ be

$$0, 0, \ldots, 0, c_k, x_{k+1}, x_{k+2}, \ldots, x_n,$$

with $k-1$ zero elements before c_k, and with

$$c_k = -\sum_{i=k+1}^{n} (x_i)^2/x_k.$$

These rows are mutually orthogonal. After row normalization the matrix can be taken as the definition of P_k in terms of the polar parameters. Sampling of the $\bar{\rho}_{kj}$, ϕ_{kj} from (5.3) or (5.4) is straightforward. In analogy to the $SU(n)$ case, if $(\bar{\rho}_{kj})^{k-2j}$ and $(2\pi)^{-1}\,\phi_{kj}$ are taken as the group parameters, then we have a mapping from $SO(n)$ to the unit hypercube in $\frac{1}{2}(n^2-n)$ dimensions such that the invariant measure is Euclidean measure on the hypercube. The mapping is continuous if the end-point values of each ϕ are identified with the same group element and if additional identifications are made when ρ_{ij} or $\bar{\rho}_{ij}$ vanish.

The extension of this formalism to $U(n)$ and $O(n)$ is routine. For $U(n)$, multiply the first row of $P_2 = (12)$ by $\exp(i\phi_0)$, where ϕ_0 is a new parameter on $(0, 2\pi)$ distributed according to $d\phi_0$. For $O(n)$, multiply the first row of $P_2 = (1\tilde{2})$ by $+1$ or -1, the two alternatives being equiprobable.

References

1. N. Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller, and E. Teller, *J. Chem. Phys.* **21** (1953), 1087.
2. M. Creutz, *Phys. Rev. D* **21** (1980), 2308; and E. Pietarinen, *Nucl. Phys. B* **190** [FS3], (1981), 349.
3. G. Guralnik, T. Warnock, and C. Zemach, *Inform. Process. Lett.* **21** (1985), 17.
4. F.·D. Murnaghan, "The Unitary and Rotation Groups," Spartan, Washington, D.C., 1962.