Sampling the eigenvalues of random orthogonal and unitary matrices

Massimiliano Fasi† Leonardo Robol‡

Abstract. We develop an efficient algorithm for sampling the eigenvalues of random matrices distributed according to the Haar measure over the orthogonal or unitary group. Our technique samples directly a factorization of the Hessenberg form of such matrices, and then computes their eigenvalues with a tailored core-chasing algorithm. This approach requires a number of floating-point operations that is quadratic in the order of the matrix being sampled, and can be adapted to other matrix groups. In particular, we explain how it can be used to sample the Haar measure over the special orthogonal and unitary groups and the conditional probability distribution obtained by requiring the determinant of the sampled matrix be a given complex number on the complex unit circle.

Key words. Random matrix, unitary matrix, orthogonal matrix, eigenvalue sampling, Haar distribution.

AMS subject classifications. 15B10, 15B52, 65F15.

1 Introduction

Random matrix theory, introduced by Wishart [36] about 90 years ago, investigates the properties of matrices whose entries are random variables. The quantities of interest range from the joint probability distribution of the matrix elements to the asymptotic behaviour of its eigenvalues and singular values [24], and applications stretch from nuclear physics [29, 35], wireless networks [10], and neuroscience [27] to numerical analysis [11, 33] and number theory [26]. Random matrix theory is still a very active area of research [28]. We refer the interested reader to the survey by Edelman and Rao [11] for a general introduction to the topic, and to the monographs by Forrester [15] and Mehta [24] for a more complete discussion. The general mechanisms by which random matrix theory can be employed to solve practical problems are discussed by Edelman and Wang [14].

†Department of Mathematics, The University of Manchester, Oxford Road, Manchester, M13 9PL, UK (massimiliano.fasi@manchester.ac.uk). The work of this author was supported by the Royal Society and the Istituto Nazionale di Alta Matematica, INdAM-GNCS Project 2019.
‡Dipartimento di Matematica, Università di Pisa, Italy (leonardo.robol@unipi.it). This author is a member of the research group GNCS, and his work has been partially supported by a GNCS/INdAM project “Giovani Ricercatori” 2018.
In applications, one is often interested in random matrices with a given structure. In quantum mechanics, for example, the energy levels of a system are described by the eigenvalue of its Hamiltonian, a Hermitian operator on an infinite-dimensional Hilbert space. By approximating this space by a Hilbert space of finite dimension, one can reduce the problem of finding the energy levels to that of solving a Hermitian eigenvalue problem. The true Hamiltonian, however, is typically not known, thus it is customary to make statistical assumptions on the distribution of its entries, enforcing only the symmetry of the operator. The distribution of the eigenvalues of random symmetric and Hermitian matrices has been extensively studied \[16, 24, 32\] and an algorithm for sampling the eigenvalues of uniformly distributed Hermitian matrices has been developed by Edelman, Sutton, and Wang \[12\].

In Section 6 we show that the empirical phase and spacing of eigenvalues sampled by our algorithm of Haar-distributed matrices from any of the Lie groups \(O(n), SU(n), U(n)\), and \(SU(n)\) are subgroups of \(O(n)\) and \(U(n)\), respectively. \(O(n)\) is made of two connected components, the already mentioned \(SO(n)\) and one in which all matrices have determinant \(-1\), which we denote by \(O^-(n)\). Clearly, the latter is not a group.

Random unitary matrices find application in quantum physics where they are employed, for example, to model scattering matrices and Floquet operators \[15, \text{Section 2.1}\]. Random orthogonal matrices, on the other hand, are used in statistical mechanics to characterize the behavior of certain log-gas systems \[15, \text{Section 2.9}\].

For a group \(G\), the measure \(\mu\) such that \(\mu(G) = 1\) is a normalized left or right Haar measure if for any \(Q \in G\) and any measurable \(\mathcal{G} \subseteq G\) it satisfies \(\mu(Q\mathcal{G}) = \mu(\mathcal{G})\) or \(\mu(\mathcal{G}Q) = \mu(\mathcal{G})\), respectively. For compact Lie groups, it can be shown that the left and right measures are unique and coincide. Hence, since \(O(n), SO(n), U(n), \text{and } SU(n)\) are all compact Lie groups \[22, \text{Chapter 1}\], they have a unique normalized (left and right) Haar measure \[23, \S\, 58, \S\, 60\].

We consider the problem of sampling efficiently the joint eigenvalue distribution of unitary (or orthogonal) matrices distributed according to the Haar measure. Numerically, this may be obtained by sampling matrices from the desired group uniformly, and then computing their eigenvalues by relying, for instance, on the QR iteration. The latter step requires \(O(n^3)\) floating-point operations (flops) to sample the \(n\) eigenvalues of a matrix of order \(n\). The key observation is that for this task it is not necessary to explicitly sample matrices from the corresponding group, but it suffices to understand the distribution of their Hessenberg forms, which we analyze in detail in Section 4. The main advantage of this approach is that unitary or orthogonal matrices in Hessenberg form can be diagonalized in \(O(n^2)\) flops. We will exploit this to derive the algorithm discussed in Section 5, which has quadratic complexity and linear storage requirements.

The algorithm we propose can efficiently sample the joint distribution of the eigenvalues of Haar-distributed matrices from any of the Lie groups \(O(n), SO(n), U(n), \text{and } SU(n)\). In Section 6 we show that the empirical phase and spacing of eigenvalues sampled by our algorithm follow the corresponding theoretical distributions for \(U(n)\), and then we explore empirically the distribution of the eigenvalues of matrices from the Haar distribution of \(SU(n), O(n), SO(n), \text{and } O^-(n)\), for which fewer theoretical results are available.

Our starting point is an algorithm proposed by Stewart \[30\] for sampling random matrices from the Haar distribution of \(O(n)\). We recall this approach and the subsequent generalization to \(U(n)\), due to Mezzadri \[25\], in Section 3. This technique exploits an algorithm for the QR
factorization based on Householder transformations, which we revise in Section 2.

These techniques require the sampling of $O(n^2)$ random variables, and need $O(n^2)$ memory for storing the result. We provide an alternative and more compact formulation for the Hessenberg form obtained by the algorithms above, which requires the sampling of $O(n)$ random variables and $O(n)$ storage. We show that this formulation can be used to compute the eigenvalues in $O(n^2)$ floating point operations by leveraging the unitary QR algorithm in [5].

The use of a condensed factorization for storing random matrices has been already explored, for instance, by Edelman and Ure [13], who sample unitary matrices by taking random Schur parameters [20]. Methods similar to the technique presented in this work might be obtained by representing the Hessenberg forms of unitary Haar-distributed matrices using Schur parameters, or similarly condensed forms such as CMV matrices [9], and then using a quadratic method to compute their eigenvalues [2, 3, 4, 6, 7, 18, 20].

The approach discussed here is based on the unitary QR algorithm in [5, Section 5], The latter can be seen as a special case of the rootfinding algorithm of Aurentz et al. [2], which has been proven to be backward stable [4], and compares favorably with the methods above in terms of performance [2].

Finally, we introduce some notation. Throughout the manuscript, we use capital letters ($A$, $B$, . . . ) to denote matrices, lower case letters ($u$, $v$, . . . ) to denote vectors, and lower case Greek letters ($\alpha$, $\beta$, . . . ) to denote scalars. We indicate the entries of matrices and vectors using a subscript notation, so that $a_{ij}$ denotes the entry in position $(i, j)$ of the matrix $A$ and $v_k$ refers to the $k$th element of the vector $v$. We use the same notation for random variables.

We denote by $N_R(p, \sigma^2)$ the Gaussian distribution centered at $\mu \in \mathbb{R}$ with variance $\sigma^2$, and by $N_R(m, n)$ the distribution of $m \times n$ random matrices with independently distributed Gaussian entries, that is,

$$X \sim N_R(m, n) \iff x_{ij} \sim N_R(0, 1), \quad i = 1, \ldots, m, \quad j = 1, \ldots, n.$$ 

The chi-squared distribution with $k$ degrees of freedom, denoted by $\chi^2(k)$, is the distribution of the sum of the squares of $k$ independent Gaussian random variables, and is formally defined by

$$\gamma \sim \chi^2(k) \iff \gamma = \sum_{i=1}^{k} \delta_i^2, \quad \delta_i \sim N_R(0, 1).$$

These are real-valued distributions. The complex counterpart of $N_R(p, \sigma^2)$ is denoted by $N_C(p, \sigma^2)$ and defined by

$$\gamma \sim N_C(p, \sigma^2) \iff \text{Re}(\gamma) \sim N_R\left(\text{Re}(\mu), \frac{\sigma^2}{2}\right) \quad \text{and} \quad \text{Im}(\gamma) \sim N_R\left(\text{Im}(\mu), \frac{\sigma^2}{2}\right).$$

The distribution $N_C^{(m, n)}$ is defined analogously.

### 2 Householder transformations and QR factorization

In this section we briefly recall some basic facts about Householder transformations, and discuss how they can be employed to compute the QR factorization of a square matrix.

Let $v \in \mathbb{C}^n$ be a nonzero vector. The matrix

$$P(v) = I_n - \frac{2}{\|v\|^2}vv^*$$

(2.1)
is a Householder transformation. It is easy to verify that \( P(v) \) is unitary and Hermitian, and in particular is orthogonal and symmetric if the entries of \( v \) are real. This implies that \( P(v)^2 = I_n \). Moreover, computing the action of \( P(v) \) on a vector requires only \( O(n) \) flops, instead of the \( O(n^2) \) flops that would be needed for a generic \( n \times n \) matrix-vector product.

Householder transformations are a convenient tool to zero out the trailing entries of a nonzero vector \( u \in \mathbb{C}^n \). For instance, let \( \theta_1 = \text{Arg} u_1 \), where \( \text{Arg} : \mathbb{C} \to (-\pi, \pi] \) denotes the principal value of the argument function. Then the matrix \( P(v) \) for \( v = u + e^{i\theta_1} \|u\|_2 e_1 \) is such that \( P(v)u = -e^{i\theta_1} \|u\|_2 e_1 \), where \( e_i \) denotes the \( i \)-th column of the identity matrix. In order to zero out only the last \( n - k - 1 \) components of \( u \in \mathbb{C}^{n \times n} \), it suffices to consider the block matrix

\[
\hat{P}_k(u) := \begin{bmatrix} I_{k-1} & P(v^{(k)}) \end{bmatrix}, \quad v^{(k)} := u^{(k)} + e^{i\theta_k} \|u^{(k)}\|_2 e_1, \quad \theta_k := \text{Arg} u_k, \quad (2.2)
\]

where \( u^{(k)} \in \mathbb{C}^{n-k} \) collects the last \( n - k \) entries of the vector \( u \).

Any matrix \( A \in \mathbb{R}^{n \times n} \) has the QR factorization \( A = QR \), where \( Q \in O(n) \) and \( R \in \mathbb{R}^{n \times n} \) is upper triangular [19, Theorem 5.2.1]. This factorization is unique up to the sign of the diagonal entries of \( R \). This result can be extended to complex matrices: any matrix \( A \in \mathbb{C}^{n \times n} \) has a unique QR factorization \( A = QR \), where \( Q \in U(n) \) and \( R \in \mathbb{C}^{n \times n} \) is upper triangular with real positive entries along the diagonal [31, Theorem 7.2]. More generally, the QR factorization of a full-rank matrix is unique as long as the phases of the diagonal entries of \( R \) are fixed.

In many of the following proofs, it will be useful to assume that the matrix \( A \) under consideration has full rank. This is typically not restrictive, since rank-deficient matrices are a zero-measure set in \( \mathcal{A}_{k,n}^{(n,n)} \) and \( \mathcal{A}_{k,n}^{(n,n)} \); we will comment on this fact in further detail when needed.

We now explain how to compute efficiently the QR factorization of an \( n \times n \) complex matrix \( A \) by means of Householder reflections [19, Section 5.2.2]. The corresponding procedure for real matrices can be obtained by employing real Householder reflectors. Let the matrix \( A^{(0)} := A \) be partitioned by columns as

\[
A^{(0)} = \begin{bmatrix} A_1^{(0)} & \cdots & A_n^{(0)} \end{bmatrix},
\]

and let \( \hat{P}_1 := \hat{P}_1(A_1^{(0)}) \). We obtain that

\[
\hat{P}_1 A^{(0)} = \begin{bmatrix} t_{11} & c \\ 0 & A_1^{(1)} \end{bmatrix}, \quad A_1^{(1)} \in \mathbb{C}^{n-1 \times n-1}, \quad c \in \mathbb{C}^{1 \times n-1},
\]

where \( r_{11} = \|A_1^{(0)}\|_2 \). If we apply this procedure recursively to the trailing submatrix \( A_1^{(1)} \), after \( n - 1 \) steps we obtain

\[
\hat{P}_{n-1} \cdots \hat{P}_1 A = R, \quad \hat{P}_k := \hat{P}_k(A^{(k-1)}), \quad k = 1, \ldots, n - 1, \quad (2.3)
\]

where the \( Q : = \hat{P}_1 \cdots \hat{P}_{n-1} \) is unitary and \( R \) is upper triangular. This algorithm produces the triangular matrix \( R \) and the factors \( \hat{P}_i \) for \( i = 1, \ldots, n - 1 \) in \( 4n^3/3 \) flops [19, Section 5.2.2]. Computing the matrix \( Q \) explicitly requires an additional \( 4n^3/3 \) flops [19, Section 5.1.6], but by exploiting the structure one can compute the action of \( Q \) on a vector or matrix with only \( n^2 \) and \( n^3 \) flops, respectively.

In order to normalize the factorization, note that if \( D \) is the diagonal matrix such that \( d_{ii} = -e^{-i\theta_i} \), where \( \theta_i \) is defined as in (2.2), then the matrix \( DR \) has positive real entries along
the diagonal. Therefore, the normalized factorization with positive diagonal entries in the upper triangular factor is:

\[
A = \tilde{Q}\tilde{R}, \quad \tilde{R} := D^*R, \quad \tilde{Q} := \tilde{P}_1\ldots\tilde{P}_{n-1}D, \quad D := -\text{diag}(e^{i\theta_1}, \ldots, e^{i\theta_n}),
\]  

(2.4)

where \(\tilde{P}_1, \ldots, \tilde{P}_{n-1}\) are as in (2.3).

A matrix \(H \in \mathbb{C}^{n \times n}\) is in upper Hessenberg form if \(h_{ij} = 0\) when \(i > j + 1\). Any square matrix is unitarily similar to an upper Hessenberg matrix, that is, for any \(A \in \mathbb{C}^{n \times n}\) there exists a matrix \(U_A \in U(n)\) such that \(U_AAU_A^*\) is an upper Hessenberg matrix. The matrix \(U_A\) can be constructed as the product of \(n - 2\) Householder transformations using a technique analogous to that discussed in this section to compute the QR factorization.

3 The Haar measure and Stewart’s algorithm

Birkhoff and Gulati [8, Theorem 4] note that if the QR factorization \(A = QR\) of an \(n \times n\) matrix \(A \sim \mathcal{N}_\mathbb{R}^{n,n}\) is normalized so that the entries along the diagonal of \(R\) are all positive, then \(Q\) is distributed according to the Haar measure over \(O(n)\).

This observation suggests a straightforward method for sampling Haar distributed matrices from \(O(n)\). One can simply generate an \(n \times n\) real matrix \(A \sim \mathcal{N}_\mathbb{R}^{n,n}\), compute its QR decomposition \(A = QR\), and normalize it as discussed in Section 2. This procedure is easy to implement, since efficient and numerically stable routines for computing the QR factorization are available in most programming languages.

The computational cost of this technique can be approximately halved by computing the QR factorization implicitly. Stewart [30] proposes an algorithm that does not explicitly generate the random matrix \(A\), but produces the transpose of the matrix \(Q\) in factored form as \(D\tilde{P}_1\ldots\tilde{P}_{n-1}\), where \(D\) is an \(n \times n\) diagonal sign matrix and \(\tilde{P}_k := \tilde{P}_k(x^{(k)})\), where \(x^{(k)} \sim \mathcal{N}_\mathbb{R}^{n,1}\).

This algorithm readily generalizes to the complex case, as discussed by Mezzadri [25]. In order to sample Haar-distributed random matrices from \(U(n)\), it suffices to generate vectors with entries drawn from the standard complex normal distribution \(\mathcal{N}_\mathbb{C}(0,1)\), and replace the real sign function \(\text{sign}(\alpha)\) by its complex generalization \(e^{i\text{Arg}(\alpha)}\).

We outline this approach in Algorithm 3.1. The function \(\text{UMULT}(X, F)\) computes the action of a Haar-distributed matrix from \(O(n)\) (if \(F = \mathbb{R}\)) or \(U(n)\) (if \(F = \mathbb{C}\)) on the rectangular matrix \(X \in \mathbb{C}^{n \times m}\). In order to determine the computational cost of the algorithm, note that asymptotically only the two matrix-vector products and the matrix sum on line 3.8 are significant. Therefore, each iteration of the for loop starting on line 3.2 requires \(4km\) flops, and the computation cost of Algorithm 3.1 is approximately \(2n^2m\) flops.

In order to sample Haar-distributed matrices, it suffices to set \(X\) to \(I_n\). In this case, the computational cost of the algorithm can be reduced by taking into account the special structure of \(A\): the cost of line 3.8 drops to \(4k^2\) flops per step, which yields an overall computational cost of \(4n^3/3\) flops.

3.1 Sampling from the special groups

The ideas presented so far can be modified in order to sample matrices with prescribed determinant. Imposing that the determinant be 1 is of particular interest, as it implies sampling from the compact Lie groups \(SU(n)\) and \(SO(n)\). As discussed in the previous section, the QR factorization of a random matrix \(A\) can be used to sample matrices distributed according to the
Algorithm 3.1: Action of a matrix from the Haar distribution.

3.1 function $\text{UMULT}(X \in \mathbb{C}^{n \times m}, F \in \{\mathbb{R}, \mathbb{C}\})$

Compute the matrix $QX$, where $Q$ is an orthogonal (if $F = \mathbb{R}$) or unitary (if $F = \mathbb{C}$) matrix from the Haar distribution.

3.2 for $k \leftarrow 2$ to $n$ do

3.3 $v \sim \mathcal{N}_F^{(k,1)}$

3.4 $d_{n-k+1} \leftarrow -e^{i \text{Arg} v_1}$

3.5 $u \leftarrow v - d_{n-k+1} \|v\|_2 e_1$

3.6 $u \leftarrow u / \|u\|_2$

3.7 $X =: \begin{bmatrix} X_1 \end{bmatrix}_{n-k}$

3.8 $X \leftarrow \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}_{k}$

3.9 $z \sim \mathcal{N}_F(0, 1)$

3.10 return $\text{diag}(d_1, \ldots, d_{n-1}, -e^{i \text{Arg} z}) \cdot X$

Haar measure over $U(n)$ and $O(n)$. An analogous result holds for the special groups, if the last diagonal entry of $R$ is chosen so that $\det Q = 1$.

Lemma 3.1. Let $A \sim \mathcal{N}_C^{(n,n)}$ (resp. $A \sim \mathcal{N}_R^{(n,n)}$) and let $A =: QR$ be its QR factorization, where $Q$ and $R$ are chosen so that

$$r_{ii} \in \{\gamma \in \mathbb{R} : \gamma \geq 0\}, \quad r_{nn} = \det(A) \cdot \left[\prod_{j=1}^{n-1} r_{jj}\right]^{-1},$$

whenever $A$ is nonsingular. Then, $Q$ is distributed according to the Haar measure over $SU(n)$ (resp. $SO(n)$).

Proof. We consider the complex case first. Note that the set of rank deficient matrices has measure zero in $\mathcal{N}_C^{(n,n)}$; therefore, the distribution of the unitary QR factor of such matrices is irrelevant for the distribution under consideration.

When $A$ is nonsingular, fixing the phases of the diagonal entries of $R$ makes the QR factorization unique. Hence, the random variables $q_{ij}$, for $i, j = 1, \ldots, n$ are well-defined. In addition, the choice of the diagonal entries of $R$ ensures that $\det R = \det A$ and thus that $\det Q = 1$.

In order to prove that $Q$ is distributed according to the Haar measure over $U(n)$, we need to show that it has the same distribution as $PQ$ for any constant matrix $P \in SU(n)$. For any such $P$, the matrix $PA$ has the QR factorization $PA =: (PQ)R$.

Being independent Gaussian random variables, the entries of $A$ are invariant under unitary transformations, thus $PA$ has the same distribution as $A$. The triangular QR factor of $PA$ is $R$, which necessarily satisfies the normalization constraints on the diagonal entries. Therefore, $PQ$ has the same distribution as $Q$.

The proof for the real case is analogous and therefore omitted. \hfill \square

The above result yields a method for sampling the Haar distribution of the special unitary and orthogonal groups. In the next sections, we discuss how to make this method efficient for
sampling the corresponding eigenvalue distribution. The approach we propose can be used for both \( U(n) \) and \( O(n) \), and \( SU(n) \) and \( SO(n) \).

**Remark 3.2.** Note that the Haar distribution of \( SU(n) \) coincides with the Haar distribution of \( U(n) \) conditioned to the event \( \det Q = 1 \). This is easily verified by checking that the latter measure is invariant under the action of elements in \( SU(n) \). This suggests that the above procedure can be further generalized and used to sample the probability \( \mu_\xi \) obtained by conditioning \( \mu \) with \( \det Q = \xi \) for some \( \xi \in S^1 \), where \( S^1 = \{ \xi \in \mathbb{C} : |\xi| = 1 \} \) denotes the complex unit circle. If \( \xi \neq 1 \), these matrices do not form a group, but we can write

\[
\{ Q \in U(n) \mid \det Q = \xi \} = \{ P\tilde{Q} \mid \tilde{Q} \in SU(n) \},
\]

where \( P \) is any constant matrix such that \( \det P = \xi \). Sampling the matrices in \( SU(n) \) and then multiplying them by any fixed \( P \) yields the correct conditional probability distribution. More specifically, by choosing the diagonal matrix \( P = \text{diag}(1, \ldots, 1, \xi) \) we can readily adapt the algorithm discussed in the next section to sample unitary or orthogonal matrices with determinant \( \xi \).

### 3.2 The eigenvalue distribution

Given a random matrix sampled according to one of the measures described so far, we are interested in describing the distribution of a generic eigenvalue. This can be computed as a marginal probability by integrating the joint eigenvalue distribution with respect to \( n - 1 \) variables. For \( U(n) \), the latter is known explicitly [24, Chapter 11], and can be used to prove that a generic eigenvalue is uniformly distributed over \( S^1 \).

We are unaware of an analogous result for \( SU(n) \), and we could not find any references stating the expected distribution for a generic eigenvalue. Nevertheless, using the fact that the eigenvalue distribution arises from Haar-distributed matrices, we can obtain the partial characterization in the following lemma. The well-known distribution for \( U(n) \) is for ease of comparison.

**Lemma 3.3.** Let \( \mu \) and \( \mu_1 \) be the Haar distributions over \( U(n) \) and \( SU(n) \), respectively, and let \( \Lambda_\mu \) and \( \Lambda_{\mu_1} \) be the corresponding distributions for a generic eigenvalue. Then, \( \Lambda_\mu \) is the uniform distribution over \( S^1 \), and \( \Lambda_{\mu_1} \) has a \( \frac{2\pi}{n} \)-periodic phase, that is,

\[
\Lambda_{\mu_1}(G) = \Lambda_{\mu_1}\left(e^{\frac{2\pi i}{n} G}\right), \quad \text{for any measurable set } G \subset S^1. \tag{3.1}
\]

**Proof.** We start considering the distribution of \( U(n) \). Recall that \( \mu \) is invariant under left multiplication in \( U(n) \), and since \( \xi I \in U(n) \) for any \( \xi \in S^1 \), we have that \( \Lambda_\mu \) is invariant under multiplication by \( \xi \in S^1 \). Being \( S^1 \) a compact Lie group, \( \Lambda_\mu \) must be its Haar measure, which is the uniform distribution.

We can use a similar argument for \( SU(n) \). Since \( \xi I \in SU(n) \) for any \( \xi \) such that \( \xi^n = 1 \), we have that \( \Lambda_{\mu_1} \) is invariant under multiplication by a root of the unity, thus must be \( \frac{2\pi}{n} \)-periodic as in (3.1).

In Section 6 we will verify this claim experimentally, to test the correctness of our implementation. In particular, we will find that \( \Lambda_\mu \) is the uniform distribution, as expected, and that \( \Lambda_{\mu_1} \) has the periodicity predicted by Lemma 3.3.
4 The Hessenberg form of Haar-distributed matrices

As mentioned in the introduction, the unitary QR algorithm of [5] cannot be applied directly to the representation of the upper Hessenberg form of a random matrix proposed by Stewart and Mezzadri. In this section, first we show how to sample a factorization of the upper Hessenberg form of Haar-distributed matrices using only $O(n)$ random variables, then we explain how to rewrite this factorization in a form that is suitable for computing the eigenvalues with core-chasing algorithms, which we briefly review in Section 5. The main result of this section is the following.

**Theorem 4.1.** Let $w_1, \ldots, w_{n-1} \in \mathbb{C}^2$ be independent random vectors such that

$$w_j = \begin{bmatrix} \alpha_j \\ \beta_j \end{bmatrix}, \quad \alpha_j \sim \mathcal{N}(0, 1), \quad \beta_j^2 \sim \chi^2(n-j),$$

and let

$$H = P_1 \cdots P_{n-1} D \in \mathbb{C}^{n \times n}$$

be the unitary Hessenberg matrix such that

$$P_j = I - \frac{2}{\|u_j\|^2} u_j u_j^*, \quad D = -\text{diag}(e^{i\theta_1}, \ldots, e^{i\theta_n}), \quad u_j = \begin{bmatrix} 0_{j-1} \\ \alpha_j + e^{i\theta_j} \|w_j\|_2 \\ \beta_j \\ 0_{n-j-1} \end{bmatrix},$$

where $\theta_j = \text{Arg} \alpha_j$ for $j = 1, \ldots, n-1$ and $\theta_n \sim U(-\pi, \pi]$. Then, the joint eigenvalue distribution of $H$ is that of Haar-distributed unitary matrices of $U(n)$.

**Proof.** In view of the discussion in Section 3, we can sample the joint eigenvalue distribution of Haar-distributed matrices by computing the eigenvalues of the unitary factor of the normalized QR factorization in (2.4), which has the form

$$Q = \tilde{P}_1 \cdots \tilde{P}_{n-1} D.$$

We now proceed to reduce the matrix $Q$ to upper Hessenberg form using similarity transformations. Let $q := Qe_1$ be the first column of $Q$ and let $U_1 = \tilde{P}_2(q)$, where the matrix $\tilde{P}_k$ is defined in (2.2). The first step of the reduction gives

$$U_1 Q U_1^* = (U_1 \tilde{P}_1 U_1^* D \tilde{D}^{-1}) U_1 \tilde{P}_2 \cdots \tilde{P}_{n-1} \tilde{D} U_1^*,$$

where $\tilde{D} = \text{diag}(1, d_{22}, \ldots, d_{nn})$. In the formula above we used the fact that $D \tilde{D}^{-1}$ commutes with $U_1$ and $\tilde{P}_2, \ldots, \tilde{P}_{n-1}$. Now note that

$$q = Q e_1 = d_{11} \tilde{P}_1 e_1 = -e^{i\theta_1} \tilde{P}_1 e_1 = -e^{i\theta_1} \left( e_1 - \frac{2u_1}{\|u_1\|^2} \right),$$

for some $u \in \mathbb{C}^n$, which implies that the first column of $Q$ depends only on $\tilde{P}_1$ and on the first entry of $D$, and that by construction the trailing $n-2$ entries of $U_1 u$ are zeros. Therefore, the matrix $P_1 := U_1 \tilde{P}_1 U_1^* D \tilde{D}^{-1}$ is of the required form (4.2). The matrix

$$U_1 P_2 \cdots P_{n-1} \tilde{D} U_1^* = \begin{bmatrix} 1 \\ \tilde{U}_1 \tilde{Q} \tilde{U}_1 \end{bmatrix},$$

where $\tilde{Q} \in \mathbb{C}^{n-1 \times n-1}$, is unitary by construction and is also Haar distributed, since $\tilde{U}_1 \in U(n-1)$ is independent of $\tilde{Q}$. The process can be repeated recursively on the smaller matrix $\tilde{U}_1 \tilde{Q} \tilde{U}_1$, and the result follows by induction. \qed
The analogue of Theorem 4.1 for real matrices is obtained by replacing the first element of $w_j$ by $\alpha_j \sim N_\mathbb{R}(0, 1)$ and by sampling $\theta_n$ uniformly from the set $\{0, \pi\}$. The result can be easily modified in order to sample the joint eigenvalues distribution of matrices from the Haar measure over $SU(n)$ and $SO(n)$: setting
\[d_{nn} = (-1)^{n-1} \prod_{i=1}^{n-1} d_{ii}\]
guarantees that $\det H = 1$, while Lemma 3.1 ensures that the matrices are sampled according to the Haar measure.

Remark 4.2. In a similar way, we may set the last diagonal entry of $D$ to obtain $\det Q = \xi$, for any $\xi \in \mathbb{S}^1$. According to Remark 3.2, this procedure samples the Haar distribution conditioned on the event $\det Q = \xi$.

5 Computing the eigenvalues of upper Hessenberg unitary matrices

By Theorem 4.1, any random upper Hessenberg unitary matrix $H$ can be described by $O(n)$ parameters by using the factored form (4.1).

The computation of the eigenvalues of unitary upper Hessenberg matrices was first considered by Gragg [20], and later investigated by numerous authors, see for instance [1, 17, 21]. Here, in particular, we are interested in the approach proposed by Aurentz, Mach, Vandebril, and Watkins [5]. This algorithm, briefly described in Section 5.2, is implemented in eiscor [3], a Fortran 90 package for the solution of eigenvalue problems by core-chasing methods available on GitHub. The software computes the eigenvalues of the Hessenberg matrix

\[H = G_1 \cdots G_{n-1} D,\]  

where the unitary matrices $G_1, \ldots, G_{n-1}$ are plane rotations of the form

\[G_j = \begin{bmatrix} I_{j-1} & \hat{G}_j & I_{n-j-1} \end{bmatrix}, \quad \hat{G}_j = \begin{bmatrix} c_j & s_j \\ -s_j & c_j \end{bmatrix}, \quad c_j \in \mathbb{C}, \quad s_j \in \mathbb{R}.\]  

Because of its special structure, the matrix $G_j$ in (5.2) is said to be “essentially $2 \times 2$”, and the $2 \times 2$ matrix $\hat{G}_j$ is called a core block. In principle, the core chasing algorithm in [5] could be applied to any factorization of $H$ involving only “essentially $2 \times 2$” unitary matrices, even though the particular implementation described in [3] involves only the special family of plane rotations. In practice, however, the key operation in the QR algorithm—the so-called turnover—has to be implemented with care in order to ensure backward stability. In order to leverage the analysis done for rotations of the form (5.2), it is thus convenient to refactorize $H$ given in the form (4.1) as a product of the the form (5.1).

This section is structured as follows. First, we show how to refactorize a representation in terms of $2 \times 2$ Householder transformations into one consisting only of plane rotations with real sines. Then we briefly recall the main ideas underlying the unitary QR algorithm implemented in eiscor.

\[\text{https://github.com/eiscor/eiscor}\]
5.1 Refactoring core transformations

The assumption that all core blocks in the factorization of the Hessenberg matrix $H$ be plane rotations with real sines is not restrictive, as it is always possible to rewrite $H$ as a product of the form (5.1). This refactorization can be performed by noting that any $2 \times 2$ unitary matrix $U$ can be written as

$$U = \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \end{bmatrix}, \quad \begin{cases} c = u_{11} e^{i\theta}, \\ s = -u_{21} e^{i\theta}, \end{cases} \quad \theta = \text{Arg}(\overline{u_{21}}),$$

where the diagonal entries are given by

$$d_1 = e^{-i\theta} |u_{11}|^2 + e^{i\theta} u_{21}^2, \quad d_2 = e^{i\theta} (u_{11} u_{22} - u_{21} u_{12}).$$

The procedure above can be performed in a backward stable manner, as it coincide with the computation of the QR decomposition of $U$ [3].

In addition, the product of a plane rotation with real sines $G$ and a unitary diagonal $2 \times 2$ matrix $D$ can be refactored so to swap the order of the two operations. In fact, there exist a unitary $2 \times 2$ diagonal matrix $\tilde{D}$ and a plane rotation with real sines $\tilde{G}$ such that $GD = \tilde{G}\tilde{D}$. This property is easy to verify, and represents the foundation of most core-chasing algorithms [3]. Combining these two observations gives the following.

**Lemma 5.1.** Let $H \in \mathbb{C}^{n \times n}$ be a unitary upper Hessenberg matrix factored as in (4.1). Then, there exist $G_1, \ldots, G_{n-1} \in \mathbb{C}^{n \times n}$ unitary plane rotations with real sines and $\tilde{D} \in \mathbb{C}^{n \times n}$ unitary diagonal such that

$$H = G_1 \ldots G_{n-1} \tilde{D}.$$  

(5.4)

This refactorization can be computed in $\mathcal{O}(n)$ flops.

**Proof.** The proof is by induction on $n$. For $n = 2$ we have that $H = P_1 D$, and the refactorization can be performed directly by relying on (5.3). If $n > 2$, then there exist a plane rotation $G_1 \in \mathbb{C}^{n \times n}$ as in (5.2) and a unitary diagonal matrix

$$D_1 := \begin{bmatrix} \alpha & \beta \\ \beta^{*} & I_{n-2} \end{bmatrix}, \quad \alpha, \beta \in \mathbb{S}^1,$$

such that $P_1 = G_1 D_1$. Since the matrix $\begin{bmatrix} d_{11} & \ldots \\ I_{n-1} \end{bmatrix}$ commutes with $D_1, P_2, \ldots, P_{n-1}$, we can write

$$H = G_1 \begin{bmatrix} d_{11} \\ I_{n-1} \end{bmatrix} \tilde{P}_2 P_3 \ldots P_{n-1} \tilde{D}, \quad \tilde{P}_2 := \begin{bmatrix} 1 & \beta \\ \beta^{*} & I_{n-2} \end{bmatrix} P_2,$$

where $\tilde{d}_{ij} = 1$ if $i = j = 1$ and $\tilde{d}_{ij} = d_{ij}$ otherwise. We note that this refactorization has the form $H = G_1 \begin{bmatrix} d_{11} \\ I_{n-1} \end{bmatrix} \tilde{H}$, where $\tilde{H}$ has the same structure as $H$ but order $n-1$. The inductive hypothesis yields $\begin{bmatrix} 1 \\ \tilde{H} \end{bmatrix} = G_2 \ldots G_{n-1} \begin{bmatrix} 1 \\ \tilde{D} \end{bmatrix}$, which gives

$$H = G_1 G_2 \ldots G_{n-1} \tilde{D}, \quad \tilde{D} := \begin{bmatrix} d_{11} \\ D' \end{bmatrix}.$$  

This procedure provides an algorithm for refactoring $H$ from the form (4.1) to the form (5.4). Noting that each step requires $\mathcal{O}(1)$ flops, for a total of $\mathcal{O}(n)$ flops for the complete refactorization, concludes the proof. □

10
5.2 Computing the eigenvalues of unitary Hessenberg matrices

We have described how to generate unitary upper Hessenberg matrices whose joint eigenvalue distribution follows the Haar measure, and we have shown how to write it in the factored form (5.4).

In order to compute the spectrum of $H$ in the form (5.4) in $O(n^2)$ flops, we rely on the method proposed in [5], which belongs to the family of core-chasing algorithms [3]. Here we provide a high-level overview of this technique, and refer the interested reader to the original paper [5] for a detailed discussion.

With the term core transformation we indicate an essentially $2 \times 2$ unitary matrix such as, for example, a plane rotation. The factorization (5.4) is an example of a matrix expressed as product of $n - 1$ core transformation and a diagonal matrix. In this particular case, the facotrization can also be used to give a compact representation of $H$ that uses only $O(n)$ parameters, as opposed to the $O(n^2)$ that would be necessary if all the entries of $H$ were explicitly stored. Each core transformation acts on a pair of adjacent indices. The matrix $G_j$ in (5.2), for example, acts on the indices $j$ and $j - 1$.

The standard single-shift bulge chasing QR algorithm works as follows. Given an upper Hessenberg matrix $H$, we determine a first core transformation $Q_1$ acting on the indices 1 and 2 such that $Q_1(H - \rho I)e_1 = \alpha e_1$. The parameter $\rho$ is the shift, and has to be carefully chosen in order to ensure fast and reliable convergence of the method [34]. The implementation considered here uses a Wilkinson shift, which is projected onto $S_1$ as the matrix $H$ is unitary [5].

We use the core transformation $Q_1$ to compute $Q_1HQ_1^*$, which is not upper Hessenberg having a nonzero element in position $(3, 1)$. Another core transformation $Q_2$ acting on the indices 2 and 3 is used to restore the upper Hessenberg structure and obtain $Q_2Q_1HQ_1^*$. The similarity $Q_2Q_1HQ_1^*Q_2^*$, however, yields a matrix that is not upper Hessenberg because of a nonzero element in position $(4, 2)$, and the process is repeated until the nonzero element, the so-called bulge, is eliminated from the last row of the matrix. The focus on the nonzero element that breaks the upper Hessenberg structure and is “chased to the bottom” until it disappears from the matrix, justifies the name bulge-chasing QR used for this algorithm.

Core-chasing algorithms have a similar formulation, and indeed are mathematically equivalent [3], but do not handle the entries of the matrix directly, as we now explain.

An upper Hessenberg matrix can always be written as $H = QR$, where $R$ is upper triangular and $Q = G_1 \ldots G_{n-1}$ is the product of unitary plane rotations. The core-chasing step starts by computing a core transformation $Q_1$ such that $Q_1(H - \rho I)e_1$ is a scalar multiple of $e_1$. Keeping $H = QR$ in factored form, the similarity transformation with $Q_1$ gives

$$Q_1HQ_1^* = Q_1G_1 \ldots G_{n-1}RQ_1^*.$$  

We now make the following two key observations.

• Given an upper triangular matrix $R$ and a core transformation $Q_1$, it is always possible to find another upper triangular matrix $\tilde{R}$ and core transformation $\tilde{Q}_1$ such that $RQ_1 = \tilde{Q}_1\tilde{R}$. Using the terminology of core-chasing algorithms, the computation of $\tilde{Q}_1$ and $\tilde{R}$ from $Q_1$ and $R$ is a passthrough operation, and can be represented pictorially as

\[
\begin{align*}
\begin{array}{ccc}
 & & \\
  & & \\
 & & \\
 & & \\
\end{array}
\end{align*}
\]
Given the matrices $G_i$ and $K_i$ acting on the $i$th and $i+1$st indices, and $J_i+1$ acting on the $i+1$st and the $i+2$nd indices, the product $G_iJ_i+1K_i$ can be refactored as $\tilde{G}_{i+1}\tilde{J}_i\tilde{K}_{i+1}$, where $\tilde{G}_{i+1}$ and $\tilde{K}_{i+1}$ act on the $i+1$st and $i+2$nd indices, and $\tilde{J}_i$ acts on the $i$th and $i+1$st indices. Similarly, this operation can be represented pictorially as

$$C_1C_1 = C_1C_1.$$  

In the context of core-chasing algorithms, it is more natural to reinterpret the refactorization above as moving the rightmost core transformation to the left, which can be displayed as

$$C_2C_2C_2.$$  

Clearly, all the rotations involved in the step above change, but from the point of view of the structure, it is as if only one rotation had moved. This operation is called turnover.

With this notation, we can rephrase the factorization obtained after introducing the core transformation $Q_1$ as

$$Q_1HQ_1^* = \begin{array}{c}
\begin{array}{c}
\begin{array}{c}
C_1C_1 \\
C_1C_1 \\
C_1C_1 \\
C_1C_1
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
R
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
C_1C_1
\end{array}
\end{array}
\end{array} = \begin{array}{c}
\begin{array}{c}
\begin{array}{c}
C_1C_1 \\
C_1C_1 \\
C_1C_1 \\
C_1C_1
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\tilde{R}
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
C_1C_1
\end{array}
\end{array}
\end{array}.$$  

In the rightmost factorization, we have first fused the top-left rotations, and then used the passthrough and turnover to take the rotation that was on the right to the left. If we call this new core transformation $Q_2$, we can now perform the similarity transformation $Q_2Q_1HQ_1^*Q_2^*$ and obtain the matrix

$$Q_2Q_1HQ_1^*Q_2^* = \begin{array}{c}
\begin{array}{c}
\begin{array}{c}
C_1C_1 \\
C_1C_1 \\
C_1C_1 \\
C_1C_1
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\tilde{R}
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
C_1C_1
\end{array}
\end{array}
\end{array}.$$  

The structure of this matrix is similar to that of $Q_1HQ_1^*$, in (5.5), but the rightmost core transformation has moved down one step. Indeed, it now acts on indices 2 and 3 instead of 1 and 2. Carrying on this process will move it further down, until it is fused at the bottom. At the very end, the core transformation will hit the bottom rotation in the sequence $G_1\ldots G_{n-1}$, and they will be fused together. This completes the chasing, and is mathematically equivalent to chasing the bulge into the bottom-right corner.

There are a few more technical details to address in order to obtain a complete algorithm. One key point is how to detect deflations, that is, eigenvalues that have converged. In the usual bulge-chasing setting, we monitor subdiagonal elements, setting them to zero as soon as they become “small enough”. For core-chasing algorithms, we observe that a subdiagonal element is small if and only if the corresponding rotation in the sequence $G_1\ldots G_{n-1}$ is close to the identity. In fact, this technique is often more accurate than the customary criterion in practice [3].

The main computational step in this process is the refactorization $RQ_1 = \tilde{Q}_1\tilde{R}$, which requires $O(n)$ flops in general. Therefore, a single core-chasing step requires $O(n^3)$ flops, and $O(n^3)$ flops will be necessary to compute the eigenvalues of a generic Hessenberg matrix, if about $O(n)$ steps...
are required for the QR iteration to converge. All the other operations require only \( O(1) \) flops, and contribute only a low-order term to the total cost.

However, if \( H \) is unitary to begin with, then so is the upper triangular matrix \( R \). As upper triangular unitary matrices must be diagonal, the passthrough operation can be performed in \( O(1) \) flops, making the cost of the QR algorithm quadratic instead of cubic in \( n \). For a more detailed analysis, we refer the reader to the paper where the algorithm was first introduced [5].

5.3 Sampling the eigenvalues of random unitary and orthogonal matrices

The approach underlying the discussion in Sections 4 and 5 is summarized in Algorithm 5.1. The function \textsc{SampleEigs} samples the joint distribution of orthogonal or unitary matrices from a specific distribution determined by the value of third parameter \( \xi \). If \( \xi = 0 \), then the function samples the eigenvalues of Haar distributed matrices from the orthogonal group, if \( \mathbb{F} = \mathbb{R} \), or from the unitary group, if \( \mathbb{F} = \mathbb{C} \). If \( \xi \neq 0 \), the algorithm samples the eigenvalue distribution of matrices whose determinant has the same phase as \( \xi \). We recall that these matrices form a group only if \( \xi = 1 \), in which case the algorithm samples the eigenvalue distribution of Haar-distributed matrices from the special orthogonal group \( \text{SO}(n) \), if \( \mathbb{F} = \mathbb{R} \), or special unitary group \( \text{SU}(n) \), if \( \mathbb{F} = \mathbb{C} \).

In order to achieve this, we note that for \( H \) in the form (5.4), we have that \( \det H = \det D = e^{i\theta} \) for some \( \theta \in (-\pi, \pi] \), since the determinant of plane rotations is 1. Therefore, once the first \( n-1 \) entries of \( D \) are chosen, it suffices to choose \( d_n = e^{i \text{Arg} \xi} d_1 d_2 \cdots d_{n-1} \), which ensures that \( \det D = e^{i \text{Arg} \xi} \). In the pseudocode, the function \textsc{UnitaryQR} denotes a call to the \texttt{eiscor} routine, which computes the eigenvalues of a product of plane rotations of the form (5.2).

The computational cost of the algorithm can be determined by noticing that each step of the for loop on line 5.3 requires only a constant number of operations, which implies that the whole preprocessing taking place between line 5.2 and line 5.18 requires only \( O(n) \) flops.

6 Experimental results

In this section we first validate the new algorithm experimentally, and then compare its performance with that of the naïve method for sampling the joint eigenvalues distribution of Haar-distributed unitary matrices. The experiments were run in MATLAB 9.8.0 (R2020a) Update 4 on a GNU/Linux machine equipped with an Intel Xeon E5-2640 v3 CPU running at 2.60GHz.

In our tests we compare the following implementations.

- \texttt{samplemat}, an algorithm that generates a Haar-distributed unitary matrix by calling the function \texttt{UMULT} in Algorithm 3.1 on the identity matrix, and then computes its eigenvalues by using the built-in MATLAB function \texttt{eig}.

- \texttt{sampleeig}, an implementation of Algorithm 5.1 that exploits the \texttt{eiscor} package to run the QR algorithm on the unitary matrix in factored form.

Our implementations of \texttt{samplemat} and \texttt{sampleeig} are available on Github.\(^2\) For reproducibility, the repository also includes the scripts we used to run the tests reported here.

\(^2\)https://github.com/numpi/random-unitary-matrices
Algorithm 5.1: Sample the joint distribution of random matrices matrices.

5.1 function SAMPLEEIGS\( (n \in \mathbb{N}, F \in \{\mathbb{R}, \mathbb{C}\}, \xi \in F) \)

Sample eigenvalues of orthogonal (if \( F = \mathbb{R} \)) or unitary (if \( F = \mathbb{C} \)) matrices. If \( \xi \neq 0 \), the determinant of the sampled matrices has the same phase as \( \xi \). If \( \xi = 0 \), the matrices are sampled from \( O(n) \) (if \( F = \mathbb{R} \)) or \( U(n) \) (if \( F = \mathbb{C} \)).

5.2 \( \delta \leftarrow 1 \)
5.3 for \( k \leftarrow 1 \) to \( n - 1 \) do
5.4 \( v_1 \sim \mathcal{N}_{\mathbb{F}}(0, 1) \)
5.5 \( v_2 \sim \sqrt{\chi^2(n-k)} \)
5.6 \( d_j \leftarrow -e^{i\text{Arg}v_1} \)
5.7 \( v_1 \leftarrow v_1 - d_j \|v\|_2 \)
5.8 \( U \leftarrow \frac{\delta}{1} (I - \frac{2}{\|v\|_2} vv^*) \)
5.9 \( \varphi \leftarrow e^{i\text{Arg} \frac{v_2}{v_1}} \)
5.10 \( c_j \leftarrow \varphi u_{11} \)
5.11 \( s_j \leftarrow -\varphi u_{21} \)
5.12 \( d_j \leftarrow d_j (\varphi |u_{11}|^2 + \varphi u_{21}^2) \)
5.13 \( \delta \leftarrow \varphi \det U \)
5.14 if \( \xi \neq 0 \) then
5.15 \( d_n \leftarrow e^{i\text{Arg} \xi - i\text{Arg}\prod_{j=1}^{n-1} d_j} \)
5.16 else
5.17 \( z \leftarrow \mathcal{N}_{\mathbb{F}}(0, 1) \)
5.18 \( d_n \leftarrow -e^{i\text{Arg} z} \)
5.19 return UNITARYQR\((c, s, d)\)

6.1 Unitary matrices

We start by considering the joint distribution of the eigenvalues of Haar-distributed matrices in \( U(n) \) and \( SU(n) \).

Figure 1 reports the phase distribution and the spacing of the eigenvalues of 1,000,000 unitary matrices of order 10 sampled from the unitary group (top row) and from the special unitary group (bottom row) using \texttt{sampleeig}. The histograms in the four plots are normalized so that the total area of the columns is one. In this way, the histograms can be interpreted as empirical probability densities and can be compared directly with the probability density functions they are expected to match.

Let \( e^{i\theta_1}, \ldots, e^{i\theta_n} \) be the eigenvalue of the matrix \( A \in U(n) \) normalized so that for \( i \) between 1 and \( n \) the phase \( \theta_i \) lies in the interval \([0, 2\pi)\). The histogram in Figure 1a shows the distribution of the phases of the 10,000,000 sampled eigenvalues, whereas the dashed lines indicates the probability density function of the uniform distribution over the interval \([0, 2\pi)\). As the eigenvalues of unitary matrices lie on the unit circle, our results indicates that the eigenvalues sampled by the procedure are uniformly distributed.

Next we investigate the statistical correlation among the eigenvalues sampled by \texttt{sampleeig}. In Figure 1b we plot the probability density function of the normalized distance between pairs
of consecutive eigenvalues, defined by
\[ \zeta_i := \frac{n}{2\pi} (\theta_{i+1} - \theta_i), \quad \theta_{n+1} := \theta_1, \quad i = 1, \ldots, n, \]
where the eigenvalues are ordered so that \( \theta_1 \leq \cdots \leq \theta_n \). In this case the dashed line represents the theoretical spacing distribution of Haar-distributed unitary matrices, known as Wigner surmise \[24, \text{Section 1.5}\]
\[ p(\zeta) = \frac{\pi \zeta}{2} \exp \left( -\frac{\pi}{4} \zeta^2 \right). \] (6.1)

The empirical distribution of the sampled eigenvalues matches closely the theoretical one, confirming that the matrices whose eigenvalues \texttt{sampleeig} samples are in fact Haar distributed.

To the best of our knowledge, the probability distribution for the phase and spacing of Haar-distributed matrices in the special unitary group are not known in closed form, but we can use \texttt{sampleeig} to obtain a relative frequency distribution based on 10,000,000 samples. The results
in Figure 1c and Figure 1d suggest that the phase of the eigenvalues of these matrices is not uniformly distributed, but the spacing appears to be the same as for Haar-distributed matrices in $U(n)$, as the empirical distribution matches the Wigner surmise in (6.1).

We note that the invariance under multiplication by elements in $SU(n)$ implies that $Q$ and $\text{diag}(\xi, \ldots, \xi)Q$ must have the same distribution for any $\xi$ such that $\xi^n = 1$, and the phase of the density of the eigenvalue distribution needs to be $2\pi/n$-periodic, as proven in Lemma 3.3. This is clearly visible in Figure 1c.

### 6.2 Orthogonal matrices

The joint eigenvalue probability density functions for $SO(n)$ and $O^-(n)$ are reported explicitly in [15, Section 2.6]. The corresponding joint eigenvalue distribution for the orthogonal group can be obtained easily, since a matrix in $O(n)$ belongs with equal probability to $SO(n)$ or $O^-(n)$. However, we are not aware of a closed form expression for the distribution of the eigenvalues of such matrices, which may be obtained by integrating out $n-1$ variables from the expressions of the joint eigenvalue distribution.

We can use `sampleeig` to get the empirical distribution of the phase and spacing of the eigenvalues of these matrices. In Figure 2, we report the relative frequency distribution of the phase and spacing of 1,000,000 random matrices of order 10 sampled from the orthogonal group (top row), from the special orthogonal group (middle row), and from the set of orthogonal matrices with determinant $-1$ (bottom row). In Figure 3 we report the same data for matrices of order 9, as the behavior of these distributions changes dramatically depending on the parity of $n$.

The distribution of phase and spacing for the eigenvalues of matrices sampled from $O(n)$ appears identical for both matrix dimensions we consider. In particular, we note that in Figure 2a and Figure 3a there is a mass of probability corresponding to the eigenvalues 1 and $-1$, which is a consequence of the fact that the eigenvalues of real matrices always appear in conjugate pairs. Therefore, if $n$ is even then matrices with determinant $-1$ must always have both eigenvalues 1 and $-1$ (see Figure 2e), whereas if $n$ is odd then all matrices with determinant 1 must have the eigenvalue 1 (see Figure 3c) and all those with determinant $-1$ must have the eigenvalue $-1$ (see Figure 3e).

### 6.3 Timings and computational complexity

Now we compare the performance of our MATLAB implementations of `sampleeig` and `samplemat`. Figure 4 shows the time, in seconds, required by the two algorithms to sample the eigenvalues of matrices of order $n$ between 2 and $2^{16}$. For matrices of order up to 16, `sampleeig` is slightly slower than `samplemat`; this is due to the fact that normalizing the rotations amounts to a large portion of the overall execution time of the algorithm. As the computational cost of this operation scales linearly, however, its contribution becomes negligible as $n$ grows: for matrices of order 32 and above the execution time grows much faster for `samplemat` than for `sampleeig`. This is expected, since the two algorithms have cubic and quadratic computational cost, respectively.

### 7 Conclusions

We have presented a method for sampling the joint distribution of the eigenvalues of Haar-distributed orthogonal and unitary matrices. The two ingredients of our approach are a tech-
Figure 2: Phase (left) and spacing (right) distribution of the eigenvalues of 1,000,000 random orthogonal matrix of order 10 sampled from the orthogonal group (top), the special orthogonal group (middle), and the connected component of the orthogonal group that contains only matrices with negative determinant (bottom) using \texttt{sampleeig}. The dashed line in the right column represent the Wigner surmise in (6.1).
Figure 3: Phase (left) and spacing (right) distribution of the eigenvalues of 1,000,000 random orthogonal matrix of order 9 sampled from the orthogonal group (top), the special orthogonal group (middle), and the connected component of the orthogonal group that contains only matrices with negative determinant (bottom) using sampleeig. The dashed line in the right column represent the Wigner surmise in (6.1).
Figure 4: Time $t_n$ (in seconds) required by `sampleeig` and `samplemat` to sample the eigenvalues of matrices of order $n$ between 2 and $2^{15}$. The tests for `samplemat` have been performed only for $n$ up to $2^{13}$.

A technique for sampling the upper Hessenberg form of Haar-distributed matrices, and an algorithm for computing the eigenvalues of an $n \times n$ upper Hessenberg unitary or orthogonal matrix in $O(n^2)$ flops.

Our experimental results show that the new technique is more efficient than the naïve method that first samples a matrix from the Haar distribution and then computes its eigenspectrum numerically. We used this algorithm to investigate experimentally the distribution of the phase and spacing of the eigenvalues of Haar-distributed matrices from $SU(n)$, $O(n)$, $SO(n)$, and $O^-(n)$, groups for which these distributions are not known explicitly.

Acknowledgments

Preparation of the manuscript was carried out, in part, while the first author was a Visiting Fellow at the University of Pisa. The authors thank Alan Edelman for providing feedback on an early draft of the manuscript.

References

[1] G. S. Ammar, L. Reichel, and D. C. Sorensen, *An implementation of a divide and conquer algorithm for the unitary eigen problem*, ACM Trans. Math. Software, 18 (1992), p. 292–307.

[2] J. L. Aurentz, T. Mach, L. Robol, R. Vandebril, and D. S. Watkins, *Roots of polynomials: On twisted QR methods for companion matrices and pencils*, arXiv:1611.02435 [math.NA], 2016.

[3] J. L. Aurentz, T. Mach, L. Robol, R. Vandebril, and D. S. Watkins, *Core-
Chasing Algorithms for the Eigenvalue Problem, Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2018.

[4] J. L. Aurentz, T. Mach, L. Robol, R. Vandebril, and D. S. Watkins, Fast and backward stable computation of roots of polynomials, part II: Backward error analysis; companion matrix and companion pencil, SIAM J. Matrix Anal. Appl., 39 (2018), p. 1245–1269.

[5] J. L. Aurentz, T. Mach, R. Vandebril, and D. S. Watkins, Fast and stable unitary QR algorithm, Electron. Trans. Numer. Anal., 44 (2015), pp. 327–341.

[6] R. Bevilacqua, G. M. Del Corso, and L. Gemignani, A CMV-based eigensolver for companion matrices, SIAM J. Matrix Anal. Appl., 36 (2015), p. 1046–1068.

[7] R. Bevilacqua, G. M. Del Corso, and L. Gemignani, Compression of unitary rank-structured matrices to CMV-like shape with an application to polynomial rootfinding, J. Comput. Appl. Math., 278 (2015), p. 326–335.

[8] G. Birkhoff and S. Gulati, Isotropic distributions of test matrices, Zeitschrift für angewandte Mathematik und Physik ZAMP, 30 (1979), pp. 148–158.

[9] M. J. Cantero, L. Moral, and L. Velázquez, Five-diagonal matrices and zeros of orthogonal polynomials on the unit circle, Linear Algebra and its Applications, 362 (2003), pp. 29–56.

[10] R. Couillet and M. Debbah, Random Matrix Methods for Wireless Communications, Cambridge University Press, Cambridge, UK, 2011.

[11] A. Edelman and N. R. Rao, Random matrix theory, Acta Numerica, 14 (2005), pp. 233–297.

[12] A. Edelman, B. Sutton, and Y. Wang, Random matrix theory, numerical computation and applications, Proceedings of Symposia in Applied Mathematics, Modern Aspects of Random Matrix Theory, 72 (2014), pp. 53–82.

[13] A. Edelman and N. K. Ure, MIT 18.338 term project: Numerical experiments on circular ensembles and Jack polynomials with Julia, 2013.

[14] A. Edelman and Y. Wang, Random matrix theory and its innovative applications, in Advances in Applied Mathematics, Modeling, and Computational Science, R. Melnik and I. S. Kotsireas, eds., no. 66 in Fields Institute Communications, Boston, 2013, Springer-Verlag, pp. 91–116.

[15] P. J. Forrester, Log-gases and random matrices, no. 34 in London Mathematical Society Monographs, Princeton University Press, Princeton, NJ, USA, 2010.

[16] Z. Füredi and J. Komlós, The eigenvalues of random symmetric matrices, Combinatorica, 1 (1981), p. 233–241.

[17] L. Gemignani, A unitary Hessenberg QR-based algorithm via semiseparable matrices, J. Comput. Appl. Math., 184 (2005), p. 505–517.

[18] L. Gemignani and L. Robol, Fast hessenberg reduction of some rank structured matrices, SIAM J. Matrix Anal. Appl., 38 (2017), p. 574–598.
[19] G. H. Golub and C. F. Van Loan, *Matrix Computations*, Johns Hopkins University Press, Baltimore, MD, USA, 4th ed., 2013.

[20] W. B. Gragg, *The QR algorithm for unitary Hessenberg matrices*, J. Comput. Appl. Math, 16 (1986), p. 1–8.

[21] W. B. Gragg and L. Reichel, *A divide and conquer method for unitary and orthogonal eigenproblems*, Numer. Math., 57 (1990), p. 695–718.

[22] B. C. Hall, *Lie Groups, Lie Algebras, and Representations*, Graduate Texts in Mathematics, Springer-Verlag, Cham, 2015.

[23] P. R. Halmos, *Measure Theory*, Graduate Texts in Mathematics, Springer-Verlag, New York, 1950.

[24] M. L. Mehta, ed., *Random Matrices*, vol. 142 of Pure and Applied Mathematics, Elsevier Academic Press, San Diego, CA, USA, 2004.

[25] F. Mezzadri, *How to generate random matrices from the classical compact groups*, Notices Amer. Math. Soc., 54 (2007), pp. 592–604.

[26] F. Mezzadri and N. C. Snaith, eds., *Recent Perspectives in Random Matrix Theory and Number Theory*, London Mathematical Society Lecture Note Series, Cambridge University Press, 2005.

[27] K. Rajan and L. F. Abbott, *Eigenvalue spectra of random matrices for neural networks*, Phys. Rev. Lett., 97 (2006).

[28] *Random matrices: The first 90 years*, J. Phys. A: Math. Theor., 52 (2018).

[29] *Special issue: Random matrix theory*, J. Phys. A: Math. Gen., 36 (2003).

[30] G. W. Stewart, *The efficient generation of random orthogonal matrices with an application to condition estimators*, SIAM J. Numer. Anal., 17 (1980), pp. 403–409.

[31] L. N. Trefethen and D. Bau III, *Numerical Linear Algebra*, Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 1997.

[32] H. F. Trotter, *Eigenvalue distributions of large Hermitian matrices; Wigner’s semi-circle law and a theorem of Kac, Murdock, and Szegö*, Adv. Math., 54 (1984), p. 67–82.

[33] J. von Neumann and H. H. Goldstine, *Numerical inverting of matrices of high order*, Bull. Amer. Math. Soc., 53 (1947), p. 1021–1100.

[34] D. S. Watkins, *The Matrix Eigenvalue Problem*, Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2007.

[35] E. P. Wigner, *On the statistical distribution of the widths and spacings of nuclear resonance levels*, Proc. Camb. Philos. Soc., 47 (1951), pp. 790–798.

[36] J. Wishart, *The generalised product moment distribution in samples from a normal multivariate population*, Biometrika, 20A (1928), p. 32.