Fast approximation of orthogonal matrices and application to PCA

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Abstract

We study the problem of approximating orthogonal matrices so that their application is numerically fast and yet accurate. We find an approximation by solving an optimization problem over a set of structured matrices, that we call Givens transformations, including Givens rotations as a special case. We propose an efficient greedy algorithm to solve such a problem and show that it strikes a balance between approximation accuracy and speed of computation. The proposed approach is relevant in spectral methods and we illustrate its application to PCA.

1 Introduction

Orthonormal transformations play a key role in most matrix decomposition techniques and spectral methods [Belabbas & Wolfe(2009)]. As such, manipulating them in an efficient manner is essential to many practical applications. While general matrix-vector multiplications with orthogonal matrices take $O(d^2)$ space and time, it is natural to ask whether faster approximate computations (say $O(d \log d)$) can be achieved while retaining enough accuracy.

Approximating an orthonormal matrix with just a few building blocks is hard in general. The standard decomposition technique meant to reduce complexity is a low-rank approximation. Unfortunately, for an orthonormal matrix, which is perfectly conditioned, this approach is meaningless.

In this work, we are inspired by the fact that several orthonormal/unitary transformations that exhibit low numerical complexity are known. The typical example is the Fourier transform with its efficient implementation as the fast Fourier transform [Van Loan(1992)] together with other Fourier-related algorithms: fast Walsh-Hadamard transforms [Fino & Algazi(1976)], fast cosine transforms [Makhoul(1980)], and fast Hartley transforms [Bracewell(1984)]. Other approaches include fast wavelet transforms [COH(1993)], banded orthonormal matrices [SIM(2007), Strang(2010)] and fast Slepian transforms [KAR(2019)]. Decomposition of orthogonal matrices into $O(d)$ Householder reflectors or $O(d^2)$ Givens rotations [Golub & Van Loan(1996)] [Chapter 5.1] are known already. In theoretical physics, unitary decompositions parametrize symmetry groups [Tilma & Sudarshan(2002)], and they are compactly parametrized using $\sigma$-matrices [Spengler et al.(2010)] or symmetric positive definite matrices [Barvinok(2006)]. To the best of our knowledge, none of these factorizations focus on reducing the computational complexity of using the orthogonal/unitary transformations but rather they model properties of physical systems.
Our idea is to approximately factor any orthonormal matrix into a product of a fixed number of sparse matrices such that their application (to a vector) has linearithmic complexity. In this paper, we derive structured approximations to orthonormal matrices that can be found efficiently and applied remarkably fast. We pose the search for an efficient approximation as an optimization problem over a product of structured matrices, that we call Givens transformations. These structures generalize Givens rotations with no computational drawback and suggest a decomposition of the main optimization problem into sub-problems that are relatively easy to understand and solved via a greedy approach. The theoretical properties of the obtained solution are characterized in terms of approximation bounds while the empirical properties are studied extensively.

We illustrate our approach considering dimensionality reduction with principal component analysis (PCA). Here the goal is not to propose a new fast algorithm to compute the principal directions, plenty of efficient algorithms for this task [Golub & Van Loan(1996)] Chapter 10 [Drineas et al.(2006), Halko et al.(2011)]. Rather, we aim at constructing fast dimensionality reduction operators. While the calculation of the principal components is a one-off computation, a numerically efficient projection operation is critical since it is required multiple times in downstream applications. The problem of deriving fast projections has also been previously studied. Possible approaches include: fast wavelet transforms [Wickerhauser(1994)], sparse PCA [Zou et al.(2006), Wang et al.(2014)], structured transformations such as circulant matrices [Jain & Haupt(2017)], Kronecker products [Kristjan H. Greenewald(2014), Givens rotations [Lee et al.(2008)], Chen & Zeng(2012)] Mathieu & LeCun(2014) or structured random projections [Ailon & Chazelle(2006), Freksen & Larsen(2017)]. Compared to these works, we propose a new way to factorize any orthogonal matrix, including PCA directions, into simple orthogonal structures that we call generalized Givens transformations and which naturally lead to optimization problems that have closed-form solutions and are therefore efficiently computed.

We end noting that our approach provides new theoretical perspectives on the structure of the orthogonal group and how to coarsely approximate it, perspectives that might have an impact on other research questions where orthogonal matrices are involved.

The paper is organized as follows: Section 2 describes the basic building blocks and algorithm that we propose, Section 3 gives the theoretical guarantees for our contributions, Section 4 details the application of our method to PCA projections and Section 5 shows the numerical experiments.

2 The proposed algorithm

Let $U$ be a $d \times d$ orthonormal matrix, then matrix-vector multiplication $Ux$ takes $O(d^2)$ operations. We want to construct $\tilde{U}$ such that $U \approx \tilde{U}$ and $\tilde{U}x$ takes $O(d \log d)$ operations. Although parametrizations of orthonormal matrices [Anderson et al.(1987)] are known, to be best of our knowledge, the problem of accurately approximating $U$ as product of only a few (less than $O(d^2)$) simple transformations is open. Then, given a $d \times p$ diagonal matrix $\Sigma_p$, we consider the problem

$$\begin{align*}
\minimize_{\tilde{U}, \tilde{\Sigma}_p} \| U \Sigma_p - \tilde{U} \tilde{\Sigma}_p \|^2_F \text{ subject to } \tilde{U} \in F_g, \\
\end{align*}$$

where $\tilde{U}$ is $d \times d$, and $\tilde{\Sigma}_p$ is a $d \times p$ diagonal matrix. Choosing $p = d$ and $\Sigma_p = \Sigma_p$ to be the identity, we simply approximate $U$. The above general formulation allow to also consider cases where different directions might have different importance. More importantly, $F_g$ is a set of orthogonal matrices–defined next– that can be applied fast and allow to efficiently solve (1).
2.1 The basic building blocks

Classic matrix building blocks that are numerically efficient include circulant/Toeplitz matrices or Kronecker products. These choices are inefficient as they depend on $O(d)$ free parameters but their matrix-vector product cost is $O(d \log d)$ or even $O(d \sqrt{d})$. Consider the sparse orthogonal matrices

$$G_{ij} = \begin{bmatrix} I_{i-1} & * & * \\ * & I_{j-i-1} & * \\ * & * & I_{d-j} \end{bmatrix}, \quad \tilde{G}_{ij} \in \left\{ \begin{bmatrix} c & -s \\ s & c \end{bmatrix}, \begin{bmatrix} c & s \\ -s & -c \end{bmatrix} \right\}, \text{ such that } c^2 + s^2 = 1,$$

(2)

where the non-zero part (denoted by * and $\tilde{G}_{ij}$) on rows and columns $i$ and $j$. The transformation in (2), with the first option in $\tilde{G}_{ij}$, is a Givens (or Jacobi) rotation. With the second option, we have a very sparse Householder reflector. These transformations were first used by [Rusu & Thompson(2017)] to learn numerically efficient sparsifying dictionaries for sparse coding. The $G_{ij}$s have the following advantages: i) they are orthogonal; ii) they are sparse and therefore fast to manipulate: matrix-vector multiplications $G_{ij}x$ take only 6 operations; iii) there are two degrees of freedom to learn: $c$ (or $s$) and the binary choice; and iv) allowing both sub-matrices in $\tilde{G}_{ij}$ enriches the structure and as we will see, leads to an easier (closed-form solutions) optimization problem.

We propose to consider matrices $\bar{U} \in \mathcal{F}_g$ that are products of $g$ transformations from (2), that is

$$\bar{U} = \prod_{k=1}^{g} G_{ikjk} = G_{i1j1} \ldots G_{igjg}.\quad (3)$$

Matrix-vector multiplication with $\bar{U}$ takes $6g$ operations – when $g$ is $O(d \log d)$ this is significantly better than $O(d^2)$, while the coding complexity of each $G_{ij}$ is approximately $2 \log_2 d + C$: $2 \log_2 d - 1$ bits to encode the choice of the two indices, a constant factor $C$ for the pair $(c,s)$ and 1 bit for the choice between the rotation and reflector. The coding complexity of $\bar{U}$ scales linearly with $g$.

We note that Givens rotations have been used extensively to build numerically efficient transformations [Lee et al.(2008)] [Cao et al.(2011)] [Kondor et al.(2014)] [Le Magoarou et al.(2018)] [Frerix & Bruna(2019)]. However, $2 \times 2$ reflector was not used before. This may be because in linear algebra (e.g. in QR factorization), or in optimization [Shalit & Chechik(2014)], considering also the reflector has no additional benefit. As we show, for our problem considering both structures have several advantages.

2.2 The proposed greedy algorithm

We propose to solve the optimization problem in (1) with a greedy approach: we keep $\tilde{\Sigma}_p$ and all variables fixed except for one (either a single $G_{ikjk}$ from $\bar{U}$ and minimize the objective function. When optimizing w.r.t. $G_{ikjk}$ it is convenient to write

$$\| U_p \Sigma_p - \bar{U} \Sigma_p \|^2_F = \| \prod_{j=1}^{k-1} G_{ijj}^T U_p \Sigma_p G_{ikjk} \prod_{j=k+1}^{g} G_{ijjj} \Sigma_p \|^2_F = \| L^{(k)} - G_{ikjk} N^{(k)} \|^2_F.\quad (4)$$

The next result characterizes the Givens transformation $G_{ikjk}$ minimizing the above norm. We drop the dependence on $k$ for ease of notation.
**Theorem 1** (Locally optimal $G_{ij}$). Let $L$ and $N$ be two $d \times p$ matrices. Further, let $Z = LN^T$ and

$$C_{ij} = \|Z_{i,j}\|_*, - \text{tr}(Z_{i,j})$$

where $Z_{i,j} = \begin{bmatrix} Z_{ii} & Z_{ij} \\ Z_{ji} & Z_{jj} \end{bmatrix}$.

Let $Z_{i^*,j^*} = V_1 S V_2^T$ be the SVD of $Z_{i^*,j^*}$, with

$$(i^*, j^*) = \arg \max_{(i,j), j > i} C_{ij}.$$  \quad (5)

Then, the Givens transformation that minimizes $\|L - G_{ij} N\|_F^2$ is $\tilde{G}_{i^*,j^*} = V_1 V_2^T$.

The above theorem derives a locally optimal way to construct an approximation $\bar{U}$. The idea is to iteratively apply the result to find for each component $k$ in (3) the Givens transformation that best minimizes the objective function (1). The full procedure is in Algorithm 1 and can be viewed in two different ways: i) a coordinate minimization algorithm; or ii) a hierarchical decomposition where each stage is extremely sparse. The proposed algorithm is guaranteed to converge, in the sense of the objective function (1), to a local minimum. Indeed, no step in the algorithm can increase the objective function, since the sub-problems are minimized exactly. We add three remarks before studying the reconstruction error of our method.

**Remark 1** (Complexity of Algorithm 1). The computational complexity of Algorithm 1 is $O(d^2 g)$ and is dominated by the computation of the scores $C_{ij}$ that takes $O(d^3)$. Note that, the $C_{ij}$s are computed from scratch only once in the initialization phase. After that, at each step $k$ we need to recompute the $C_{ij}$ (redo the $2 \times 2$ singular value decompositions) only for the indices $(i_k, j_k)$ currently used (the Givens transformations act on two coordinates at a time). All other scores are update by the same quantity: in (5), the $C_{ij}$ stay the same by the trace term changes due to the operations on $(i_k, j_k)$. This observation substantially reduces the running time.

**Remark 2** (Complexity of applying $\bar{U} \Sigma_p$). When $p < d$ the computational complexity of $6g$ operations is an upper bound. Since we keep only $p$ components, we need be careful not to perform operations whose result is thrown away by the mask $\Sigma_p$. Consider for example a transformation $G_{1d}$ applied to a vector of size $d$ projected to a $p < d$ dimensional space. The three operations that take place on the $d$th component are unnecessary. Then, after computing $\bar{U}$, a pass is made through each of the $g$ transforms to decide which of two coordinates the computations are necessary for the final result. As we will show, this further improves the numerical efficiency of our method.

**Remark 3** (On the choice of indices). Algorithm 1 greedily chooses at each step $k$ the indices according to (5). Other factors might be considered: i) choosing indices based on previous choices so that only a select group of indices are used throughout the algorithm, or ii) make multiple choices at each step in order to speed up the algorithm.

### 3 Analysis of the proposed algorithm

We consider $p = d$, i.e., $\Sigma_p = I_{d \times d}$ and therefore $Z = U$. We model the $U$ as a random orthonormal matrix with Haar measure updated so that the diagonal is positive. We perform this update because multiplication by a diagonal matrix with $\pm 1$ entries has no computational cost but it brings $U$ closer to $I_{d \times d}$. The goal of this section is to establish upper bounds for the distance between $U$ and $\tilde{U}$, as a function of $d$ and $g$. We first comment on the inherent difficulty of the problem.
Algorithm 1 Approximate orthonormal matrix factorization with Givens transformations

Input: The $p$ orthogonal components $U_p$ and their weights (singular values) $\Sigma_p$, the size $g$ of the approximation [3] and the update rule for $\Sigma_p$ {‘identity’, ‘original’, ‘update’}.

Output: The linear transformation $\bar{U}\bar{\Sigma}$, the approximate solution to (1).

Initialize: $G_{i_k, j_k} = I_{d \times d}, k = 1, \ldots, g$ and compute all scores $C_{ij}$ according to (5) with $Z = U_p\Sigma_p^T$, where $\Sigma_p = [I_p \times p; \ 0_{(d-p) \times p}]$ if the update rule is ‘identity’ and $\Sigma_p = \Sigma_p$ otherwise.

repeat
  Set $L^{(0)} = U_p$ and set $N^{(0)} = G_{i_1, j_1} \ldots G_{i_g, j_g} M$.
  for $k = 1$ to $g$ do
    Update $N^{(k)} = G_{i_k, j_k}^T N^{(k-1)}$ and find best score according to (5).
    Compute the best $k$th transformation by Theorem 1.
    Update $L^{(k)} = G_{i_k, j_k}^T L^{(k-1)}$ and then update all scores $C_{ij}$ in (5) with $Z = L^{(k)}(N^{(k)})^T$.
  end for
  Set $\Sigma_p = [\text{diag}(L^{(g)}); \ 0_{(d-p) \times p}]$ if rule is ‘update’, $i \leftarrow i + 1$ and $\epsilon_i = \|L^{(g)} - \Sigma_p\|^2_F$.
until $|\epsilon_{i-1} - \epsilon_i| < \epsilon$, if $i > 1$.

Remark 4 (The approximation gap). Since the orthogonal group has size $O(d^2)$, by the pigeonhole principle a random orthogonal matrix as [3] and only $g \ll d^2$ degrees of freedom cannot be exactly approximated with less than $O(d^2)$ operations. For our purposes, think $g$ either $O(d)$ or $O(d \log d)$. Our goal is to show that the fast structures we propose can perform well in practice and have theoretical bounds that guarantee worse case or average accuracy.

Next, we discuss two approximations bounds depending on the number of Givens transformations.

Theorem 2 (A special bound). Given a random $d \times d$ orthonormal $U$ its approximation $\bar{U}$ from [1] with $g = d/2$ transformations [2] obeys
\[
\mathbb{E}[\|U - \bar{U}\|^2_F] \leq 2d - \sqrt{2\pi d}.
\] (6)

Theorem 3 (A general bound). Given a random $d \times d$ orthonormal $U$ its approximation $\bar{U}$ from [1] with $g \leq (d-1)/2$ transformations [2] is bounded by
\[
\mathbb{E}\left[\|U - \bar{U}\|^2_F\right] \leq 2(d - |r|) - \frac{2\sqrt{2}}{\sqrt{\pi}} \sqrt{d - |r|}, \quad \text{where } r = d - \frac{1 + \sqrt{(2d - 1)^2 - 8g}}{2}.
\] (7)

Theorem 2 shows that, on average, the performance might degrade with increasing $d$. As stated in Remark 4, this is not surprising since the orthonormal group is much larger than the structure we are trying to approximate it with. The next result provides a bound for other values of $g$. In Theorem 3, taking $g = c_1 d \log d$ for some positive constant $c_1$ we have that $r \approx c_1 \log d$. This means that whenever $p \ll d$ we will roughly need $O(d)$ Givens transformations to improve the $|r|$ term. Since the proof of the theorem uses only rotations (and furthermore, in a particular order of indices $(i_k, j_k)$) we expect our algorithm to perform much better than the bound indicates as it allows for a richer structure [2] and uses greedy steps that maximally improve the accuracy at each step.

The previous theorems consider the Frobenius norm. In the Jacobi iterative process for diagonalizing a symmetric matrix with Givens rotations [Golub & Van Loan (1996) Chapter 8.4] the progress of the procedure (convergence) is measured using the off-diagonal “norm” off($U$) = $\sqrt{\sum_i \sum_{q \neq i} U_{iq}^2}$. 

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Then, by direct calculation we have that

\[
\text{off}(UG^T) = \text{off}(U) + \frac{1}{2}((U_{ii} - U_{jj})^2 - (U_{ij} - U_{ji})^2).
\]

This result shows that, unlike with the Jacobi iterations, monotonic convergence in this quantity is not guaranteed and depends on the relative differences between the diagonal and the off-diagonal entries of $U_{i,j}$. Our method convergence monotonically when we measure the progress in the Frobenius norm.

**Remark 5** (The effect of a single $G_{ij}$). Given a $d$ $d$ orthonormal $U$ and a Givens transformation $G_{ij}$ we have that: i) $UG_{ij}^T$ is closer to the identity matrix in the sense that $G_{ij}$ makes a positive contribution to the diagonal elements, i.e., $\text{tr}(UG_{ij}^T) = \text{tr}(U) + C_{ij}$; and ii) $E[C_{ij}] \approx 0.6956d^{-1/2}$ if $U$ is random, with Haar measure and positive diagonal.

The above remark suggests a metric to study the convergence of the proposed method: each Givens transformation adds the score $C_{ij}$ to the diagonal entries of the current approximation (and therefore ensures that $U\bar{U}^T$ converges to the identity – the only diagonal orthonormal matrix). By choosing the maximum $C_{ij}$ we are taking the largest step in this direction.

**Remark 6** (Evolution of $C_{i,k}$ with $k$). Given a fixed $0 < u < 1$, consider the toy construction $U_{i,j} = \begin{bmatrix} u & z_2 \\ z_1 & u \end{bmatrix}$, i.e., for a $d$ $d$ matrix with diagonal elements equal and off-diagonals two independent uniform random variables in the interval $[-\sqrt{1-u^2}, \sqrt{1-u^2}]$ (since rows and columns of $U$ are $\ell_2$ normalized). Then, by direct calculation we have that $E[C_{ij}(u)]$ (the $C_{ij}$ as a function of $U$) obeys

\[
E[C_{ij}(u)] \approx (1-u)^2,
\]

i.e., the expected $C_{ij}$ decreases on average quadratically with the increase in the diagonal elements.

The remark is intuitive: as $k$ increases $\bar{U}$ is more accurate and $U\bar{U}^T$ becomes diagonally dominant ($U\bar{U}^T \to I_d$ as $k \to O(d^2)$) and we do expect to reach lower scores $C_{i,k}$, i.e., few Givens transformations provide a rough estimation while very good approximations require $k \approx d^2$.

Proofs of the results and details on remarks are collected in the attached supplementary materials.

### 4 Application: fast PCA projections

Consider a training set of $d$-dimensional points $\{x_i\}_{i=1}^N$ and the $d \times N$ matrix $X = [x_1 \ldots x_N]$. Given $1 \leq p < d$, PCA provides the optimal $p$-dimensional projection that minimally distorts, on average, the data points. The projection is given by the eigenvectors of the $p$ largest eigenvalues of $XX^T$ or, equivalently, the left singular vectors of the $p$ largest singular values of $X$, that is

\[
XX^T \approx U_p\Sigma_p\Sigma_p^TU_p^T \quad \text{and} \quad X \approx U_p\Sigma_pV_p^T.
\]

Given the above decompositions we can approximate $X$ by $\bar{X} = \bar{U}\Sigma_pV_p^T$, i.e., we keep $V_p$ but we modify the principal components and their singular values, such that we minimize the error given by

\[
\|U_p\Sigma_pV_p^T - \bar{U}\Sigma_pV_p^T\|_F^2 = \|U_p\Sigma_p - \bar{U}\Sigma_p\|_F^2.
\]
where $U_p$ is $d \times p$, the diagonal matrix $\Sigma_p$ is $p \times p$, $\bar{U}$ is of size $d \times d$, $\Sigma_p$ is $d \times p$ and is zero except for its main $p \times p$ diagonal. In this paper, we work with $X$, as opposed to $XX^T$, to keep the relationship with $U_p$ linear, rather than quadratic. In the context of applying our approach to PCA, we use our decomposition on the principal components $U_p$ which we assume are already calculated together with the associated singular values $\Sigma_p$ which we may use as weights in (1).

Note that in (11), $V_p$, which has size $N$, is not necessary and that the two-step procedure is equivalent to computing the projections $\bar{U}$ directly from $X$. Also note that based on (10), we could factor $X \approx \bar{U} \Sigma \bar{V}^T$ where $\bar{U}$ and $\bar{V}^T$ are approximations in $F_{O(d \log d)}$ and $F_{O(N \log N)}$, respectively. The difficulty here is the dependency of $\bar{V}$ on $N \gg d$ which would require a large running time. With $\bar{U}$ fixed, for $\Sigma_p$ we have several strategies: i) set it to the identity, i.e., flatten the spectrum; ii) keep it to the original singular values $\Sigma_p$; or iii) continuously update it to minimize the Frobenius norm, i.e., get the new "singular values" that are optimal with the approximation $\bar{U}$. The first approach favors the accurate reconstruction of all components while the other approach favors mostly the few leading components only (depending on the decay rate of the corresponding singular values).

4.1 Comparison with the symmetric diagonalization by Givens rotations approach

Because of the locally optimal way the Givens transformations are chosen (see Theorem 1), our proposed factorization algorithm is computationally slower than the Jacobi diagonalization process which chooses the Givens rotations on indices $(i,j)$ corresponding to the largest off-diagonal entry of the covariance matrix. Furthermore, the Jacobi decomposition uses each rotation to zero the largest absolute value off-diagonal entry and because of this sub-optimal choice needs $O(d^2 \log d)$ Givens rotations [Brent & Luk(1985)] to complete de diagonalization (more than the $\frac{d(d-1)}{2}$ needed to fully represent the orthonormal group).

In all other aspects, our approach provides advantages over the Jacobi approach: i) we define a clear objective function that we locally optimize exactly; ii) it is known that the Jacobi process converges slowly when the number of rotations is low [van Kempen(1966)], which is exactly the practically relevant scenario we have, i.e., $g \ll d^2$; iii) with the same computational complexity, i.e., $g$ terms in the factorization, our proposed approach is always more accurate since we include as a special case the Givens rotations.

4.2 Comparison with structured matrix factorization

Our approach requires the explicit availability of the orthonormal principal directions $U_p$. Previous methods that factor using only Givens rotations are not applied directly on an orthogonal matrix. These methods rely on receiving as input a symmetric object (e.g., $XX^T$) and then using a variant of Jacobi iterations for matrix diagonalization [Le Magoarou et al.(2018)] or multiresolution factorizations [Kondor et al.(2014)] to find the good rotations that approximate the orthonormal eigenspace. Applying Givens transformations directly to $X$ on the left, i.e., $G_{ij}X$, cannot lead to the computation of the PCA projections $U$ but only to the polar decomposition. On the other hand, when applying Givens rotations on both sides of the covariance matrix, i.e., $G_{ij}XX^T G_{ij}^T$, then the right eigenspace $V$ cancels out in the product (10) and we are able to directly recover $U$ (but we need $XX^T$ explicitly). Finally, note that the diagonalization process approximates the full eigenspace $U$ and cannot separate from the
start the \( p \) principal components \( U_p \) because they are solving the following problem

\[
\minimize_{\bar{U}, \bar{A}} \|XX^T - \bar{U}\bar{A}\bar{U}\|^2_F \text{ subject to } \bar{U} \in F_g.
\] (12)

This formulation is useful to approximate the whole symmetric matrix \( XX^T \) (or \( U \)), but not necessarily the \( p \) principal eigenspace \( U_p \). To get these we would need to complete the diagonalization process, find the \( p \) largest entries on the diagonal of \( \bar{A} \) and then work backward to identify the rotations that contributed diagonalizing those largest elements. This procedure would be prohibitively expensive. Previous work, e.g. [Lee et al.(2008), Kondor et al.(2014)], deals with approximating \( XX^T \) rather than computing PCA.

5 Experimental results

Given the rather pessimistic guarantees, we tackle problems: how well does Algorithm 1 recover random orthogonal matrices and principal components such that we benefit from the computational gains but do not significantly impact the approximation/classification accuracy. Source code available.

5.1 Synthetic experiments

For fixed \( d \) we generate random orthonormal matrices from the Haar measure [Johansson(1997)]. Figure 1 shows the representation error \( (2d)^{-1}\|U - \bar{U}\|^2_F \) for the proposed method. The plot shows that allowing for the Givens transformations \( \tilde{G}_{ij} \) in (2) brings a 17% relative benefit as compared to using only the Givens rotations while, for the same \( g \), the computational complexity is the same. The circulant approximation performs worst because it has the lowest number of degrees of freedom, only \( d \) (computationally, it is comparable with the Givens and proposed approaches for \( g = 100 \)). Lastly, we can observe that the bound is very pessimistic, especially for these values of \( g \).

5.2 MNIST digits and fashion

We now turn to a classification problem. We use the MNIST digits and fashion datasets. The points have size \( d = 400 \) (we trimmed the bordering whitespace) and we have \( N = 6 \times 10^4 \) training and \( N_{\text{test}} = 10^4 \) test points. In all cases, we use the k-nearest neighbors (k-NN) algorithm with \( k = 10 \), and we are looking to correctly classify the test points. Before k-NN we apply PCA and our proposed method. Results are shown in Figure 2. We deploy two variants of the proposed method: approximate the principal components as if they had equal importance and approximate the principal components while simultaneously also updating estimates of the singular values.

For comparison, we also show the sparse JL [Kane & Nelson(2014)]. In this case, the target dimension is \( p \in \{15, 30\} \) while the random transformation of size \( p \times d \) only has three non-zero entries per column. More non-zeros did not have any significant effect on the classification accuracy while increasing (doubling, in this case) the target dimension \( p \) increases the classification accuracy by 10%. The results reported in the plots are averages for 100 realizations and the standard deviation is below 1%. Of course, the significant advantage of the JL approach over PCA is that no training is needed. The disadvantage is that if we choose greedily the target projection dimension, i.e., low \( p \), the accuracy degrades significantly for JL. Results are identical for PCA when \( p \) is 15 of 30.

\footnote{https://github.com/cristian-rusu-research/fast-orthonormal-approximation}
Since we are dealing with image data, we also project using the discrete cosine transform (DCT). For the digits dataset, the performance is poor but, surprisingly, for the fashion dataset, this approach is competitive given the large speedup it reports (we used the sparse fast Fourier transform [Indyk et al. (2014)] as we want only the largest \( p \) components). We have also performed the projection by fast wavelet transforms with ‘haar’ and several of the Daubechies ‘dbx’ filters but the results were always similar to that of the DCT. For clarity of exposition, we did not add these results to the figures. Our proposed methods report a clear trade-off between the classification accuracy and the numerical complexity of the projections. If we insist on an accuracy level close (within 1–2\%) of the full PCA then the speedup is only about \( x3 \). Reasonable accuracy is obtained for a speedup of \( x4\)–\( x5 \) after which the results degrade quickly. For \( p = 15 \) better performance seems impossible via randomization.

Finally, in Figure 2 (left) we compare our proposed methods against the sparse PCA on MNIST digits. sPCA performs exceptionally well in terms of the classification accuracy given the computational budget (a similar result is replicated for MNIST fashion). On other datasets where the principal components capture some global features (not local like in our example) we expect this performance to degrade. The training time of sPCA exceeds by 60\% the running time of PCA plus that of our method. We used the implementation [Wang et al. (2014)]. Because of ideas in Remark 1, we perform only the finally useful calculations and further reduce the computational cost on average by one third (these are accounted for already in the numbers in the plots).

5.3 Experiments on other datasets

The 20-newsgroups dataset consists of 18827 articles from 20 newsgroups (approximately 1000 per class). The dataset was tokenized using the rainbow package. Each article is represented by a word-count vector for the \( d = 2 \times 10^4 \) common words in the vocabulary. For this dataset we have \( N_{\text{test}} = 5648 \), \( p = 200 \), and as shown in Figure 3 (right) in this case we outperform sparse PCA.

We also apply our algorithm to several other popular dataset from the literature: PENDIGITS with 10 classes and \( d = 16 \), \( N = 7494 \), \( N_{\text{test}} = 3498 \), \( p = 4 \); ISOLET with 26 classes and \( d = 617 \), \( N = 6238 \),
Table 1: Average classification accuracies for k-NN when using PCA projections and our approximations without spectrum update, for various datasets. We also show the speedup and the number of features selected in the calculations as a proportion out of the total $d$ (see also Remark 2).

| Dataset       | Full PCA Accuracy | Proposed Accuracy | Accuracy/Speedup/Selection |
|---------------|-------------------|-------------------|-----------------------------|
| PENDIGITS     | 95 ± 0.7          | 91 ± 2.1          | 1.6 / 1                     |
| ISOLET        | 92 ± 0.4          | 90 ± 1.0          | 12 / 1                      |
| USPS          | 95 ± 1.2          | 94 ± 0.8          | 7.7 / 0.64                  |
| UCI           | 90 ± 1.9          | 87 ± 1.5          | 2.5 / 0.72                  |
| 20NEWS        | 80 ± 3.1          | 77 ± 2.1          | 3.1 / 0.3                   |
| EMNIST digits | 97 ± 2.5          | 95 ± 1.8          | 13 / 0.37                   |
| MNIST 8M      | 96 ± 2.0          | 94 ± 0.9          | 15 / 0.28                   |

Figure 3: Classification accuracy versus number of operations on the MNIST digits (left) and 20NEWS (right) datasets for our proposed methods and the sparse PCA method [Zou et al.(2006), Wang et al.(2014)].

Figure 4: A few eigenfaces obtained by the optimal PCA (top) and by our proposed method with $g = 3059$ and $g = 1020$ (middle and bottom, respectively). The projection speedup is x4.1 and x13.9, respectively.

$N_{\text{test}} = 1559$, $p = 150$; USPS with 10 classes and $d = 256$, $N = 7291$, $N_{\text{test}} = 2007$, $p = 12$; UCI with 10 classes and $d = 64$, $N = 3823$, $N_{\text{test}} = 1797$, $p = 6$; EMNIST digits with 10 classes and $d = 784$, $N = 24 \times 10^4$, $N_{\text{test}} = 4 \times 10^4$, $p = 15$; MNIST 8m with 10 classes and $d = 784$, $N = 6.4 \times 10^6$, $N_{\text{test}} = 1.7 \times 10^6$, $p = 15$. All the results are shown in Table 1.

One of the most famous applications of PCA is in the field of computer vision for the problem of human face recognition. The eigenfaces [Sirovich & Kirby(1987)] approach was used successfully for face recognition and classification tasks. Here, we want to reproduce the famous eigenfaces by using the proposed methods. The original eigenfaces and their approximations (sparse eigenfaces [Zhang et al.(2014)]), with different $g$ and therefore different levels of detail, are shown in Figure 4.

6 Conclusions

This paper proposes a new matrix factorization algorithm for orthogonal matrices. The key ingredient is a class of structured matrices, called Givens transformations. We show that there is a trade-off between the computational complexity and accuracy of the approximations created by our approach. We apply our method to the approximation of a fixed number of principal components and show that,
with a minor decrease in performance, we can reach significant computational benefits. Future research directions include strengthening the theoretical guarantees since they are way above what we observe experimentally. Further, it would be of interest to improve the complexity of the proposed algorithm either by a parallel implementation or using randomization (e.g. computing a random subset of the $O(d^2)$ scores). As an application, it would be interesting to apply our decomposition to the recently proposed unitary recurrent neural networks [Wisdom et al. (2016)].

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Supplementary materials

More on Remark 3. We say that the orthonormal group has $O(d^2)$ degrees of freedom as it was established [Anderson et al. (1987)] that any orthonormal matrix $U$ can be factored into a product as

$$U = \left( \prod_{i=1}^{d} \prod_{j=i+1}^{d} G_{ij}(\theta_{ij}) \right) D,$$  \hspace{1cm} (13)

where $D$ is a diagonal matrix with entries only in $\{\pm 1\}$ and the $G_{ij}(\theta_{ij})$ are Givens rotations, with angles $\theta_{ij}$, i.e., we have $c = \cos \theta_{ij}$ and $s = \sin \theta_{ij}$ in [2]. To generate a random orthonormal $U$ we therefore need to generate random $D$ (which are $\{\pm 1\}$ with equal probability) and $\frac{d(d-1)}{2}$ random angles $0 \leq \theta_{ij} \leq \pi/2$. These angles are mutually independent and It is known that their joint density function is a random variable

$$Z \propto \left( \prod_{k=2}^{d} \cos^{k-2} \theta_{1k} \right) \left( \prod_{k=3}^{d} \cos^{k-3} \theta_{2k} \right) \left( \prod_{k=d}^{d} \cos^{d-\theta_{(d-1)k}} \right).$$  \hspace{1cm} (14)

We define the beta random variable $\sqrt{y} = \cos \theta$ (and $\pm \sqrt{1-y} = \sin \theta$) with density

$$f(y, \alpha, \beta) = \frac{y^{\alpha-1}(1-y)^{\beta-1}}{B(\alpha, \beta)}, \quad B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)} \text{ with } y \in [0,1].$$  \hspace{1cm} (15)

Because we are interested in the computational complexity of a random orthonormal matrix we focus on the following three special cases: i) do nothing: $\tilde{G}_{ij} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$; ii) permute coordinates: $\tilde{G}_{ij} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$; and iii) $\tilde{G}_{ij} \in \left\{ \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}, \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \right\}$. The first two cases perform no operations while the last performs only 4 (as compared to 6 for a general rotation). Unfortunately, the joint density in [14] does not seem to have a closed form expression. As such we show in Figure 5 numerical results of the probability distribution of $\cos \theta$ over all angles $\theta_{ij}$, which we observe numerically that approaches an exponential distribution $\lambda \exp(-\lambda c)$. Concentration around the three special cases does not occur and therefore a random orthonormal matrix will generally have computational complexity $O(d^2)$. For example, if we discretized the continuum of $c = \cos \theta$ then the probability that a random $U$ is an approximate permutation matrix and therefore basically exhibits no numerical complexity is $\left( 1 - \exp(-\lambda c) \right)^{d(d-1)/2}$ for $0 < \epsilon \ll 1$, i.e., the probability that all $\frac{d(d-1)}{2}$ rotations have $\cos \theta \leq \epsilon$. □

Proof of Theorem 1. For simplicity of exposition we will drop the sub-index $k$ herein and therefore [4] develops to the following

$$\|L - G_{ij}N\|_F^2 = \|L\|_F^2 + \|G_{ij}N\|_F^2 - 2\text{tr}(N^TG_{ij}^TL) = \|\sigma_p\|_2^2 + \|\bar{\sigma}_p\|_2^2 - 2\text{tr}(G_{ij}^TLN^T),$$  \hspace{1cm} (16)

where the Frobenius norms reduces to the $\ell_2$ norms of the spectra and we have used the circular permutation property of the trace. It is convenient to denote $Z = LN^T$ and the $2 \times 2$ matrix $Z_{(i,j)} = \begin{bmatrix} Z_{ii} & Z_{ij} \\ Z_{ji} & Z_{jj} \end{bmatrix}$. Given that $G_{ij}$ performs operations only on rows $i$ and $j$, the trace is

$$\text{tr}(G_{ij}^TLN^T) = \sum_{k=1, k \notin \{i,j\}}^d Z_{kk} + \text{tr}(\tilde{G}_{ij}Z_{(i,j)}) = \text{tr}(Z) + \text{tr}(\tilde{G}_{ij}Z_{(i,j)}) - \text{tr}(Z_{(i,j)}).$$  \hspace{1cm} (17)
Figure 5: Experimental distribution on the entries (cosine and sine on the left and right, respectively) of the Givens rotations $G_{ij}$ from [13]. We observe numerically that $\cos \theta$ follows closely an exponential distribution $\lambda \exp(-\lambda c)$ with $\lambda \approx \sqrt{d}/2$ on the interval $[0,1]$.

To minimize the quantity in (16) we have to maximize (17) which is known as a Procrustes problem [Schonemann(1966)] whose solution is given by the polar decomposition of $Z_{ij}$ detailed in [Golub & Van Loan(1996)] Chapter 9.4.3. Therefore, we set the optimal transformation to

$$\tilde{G}_{ij}^* = V_1V_2^T, \quad Z_{ij} = VSV_2^T,$$  \hspace{1cm} (18)

where use the SVD of $Z_{ij}$ ($S = \text{diag}(s_1, s_2)$ are the singular values). With this choice, we have

$$\max \text{tr}(G_{ij}^T LN^T) = \text{tr}(Z) + \text{tr}(S) - \text{tr}(Z_{ij}) = \text{tr}(Z) + ||Z_{ij}||_* - \text{tr}(Z_{ij}) = \text{tr}(Z) + C_{ij}. \quad (19)$$

We denote the nuclear norm $||Z_{ij}||_*$, i.e., the sum of the singular values $s_1$ and $s_2$ and we define

$$C_{ij} = ||Z_{ij}||_* - \text{tr}(Z_{ij}). \quad (20)$$

Intuitively, the results (16), (17) follows after observing that: 1) the $G_{ij}$ can be viewed as a perturbed identity matrix; 2) if $G_{ij}$ is exactly $I_{d \times d}$ then $||L - N||_F^2 = ||\sigma_p||^2 + ||\bar{\sigma}_p||^2 - 2\text{tr}(Z)$ while if $G_{ij}$ is the optimal orthonormal transformation $Q$ that minimizes (16) given by the Procrustes solution [Schonemann(1966)] then we have $||L - QN||_F^2 = ||\sigma_p||^2 + ||\bar{\sigma}_p||^2 - 2||Z||_*$, where the last term is the nuclear norm of $Z$; 3) therefore, we actually apply the identity transformation on all coordinates, i.e., the tr($Z$) term, while for the two chosen coordinates we apply the best (in the sense of reducing the error) orthogonal transformation whose contribution is the nuclear norm term $||Z_{ij}||_*$ and then correct for the trace term that was wrongly added initially in tr($Z$), by subtracting tr($Z_{ij}$).

There are $d(d-1)/2$ quantities $C_{ij}$ but they can be computed efficiently by noting that in the $2 \times 2$ case the singular values of $Z_{ij}$ are $s_{1,2} = \sqrt{\frac{1}{2}} \left( ||Z_{ij}||_F^2 \pm \sqrt{||Z_{ij}||^4_F - 4 \det(Z_{ij})^2} \right)$. \hspace{1cm} ■

**Proof of Theorem 2.** Assume $d$ is even and partition the set $\{1, \ldots, d\}$ into $d/2$ pairs of indices $(i_k, j_k)$. We therefore have

$$\frac{d}{2} \sum_{k=1}^{d/2} C_{i_kj_k} = \frac{d}{2} \sum_{k=1}^{d/2} (||U_{i_kj_k}||_* - U_{i_ki_k} - U_{j_kj_k}) = \sum_{k=1}^{d/2} ||U_{i_kj_k}||_* - \text{tr}(U). \quad (21)$$

As a side note, to maximization of this partitioned quantity is related to the weighted maximum matching algorithm (of maximum-cardinality matchings) on the graph with $d$ nodes and with edge
weights \( C_{ik,jk} \). With this choice of indices, the objective function becomes

\[
\| U - \prod_{k=1}^{d/2} G_{ik,jk} \|_F^2 = 2d - 2\text{tr}(U) - 2 \sum_{k=1}^{d/2} C_{ik,jk} = 2d - 2 \sum_{k=1}^{d/2} \| U_{ik,jk} \|_*,
\]  

(22)

We use the singular value decomposition of a generic \( U_{i,j} = V_1 S V_2^T \), \( S = \text{diag}(s) \), and develop:

\[
|\text{tr}(U_{i,j})| = |\text{tr}(V_1 S V_2^T)| = |\text{tr}(S V_2^T V_1)| = |\text{tr}(S \Delta)| = \sum_{t=1}^{2} s_t |\Delta_{tt}| \leq \Delta_{\text{max}} \sum_{t=1}^{2} s_t = \Delta_{\text{max}} \| U_{i,j} \|_*,
\]

(23)

where we have use the circular property of the trace and \( \Delta = V_2^T V_1 \) where \( \Delta_{tt} \) are its diagonal entries which obey \( |\Delta_{tt}| \leq \Delta_{\text{max}} \). We define the diagonal coherence as

\[
\Delta_{\text{max}} = \max\{|\Delta_{11}|, |\Delta_{22}|\}.
\]

(24)

With (23), we can state that for the \( k \)-th transformation that

\[
\mathbb{E}[\| U_{ik,jk} \|_*] \geq \frac{\pi}{2} \mathbb{E}[\text{tr}(U_{ik,jk})],
\]

(25)

where we have used the fact that \( V_1 \) and \( V_2 \) have the structure \( G_{ij} \) in (2) and therefore

\[
\mathbb{E}[\Delta_{\text{max}}] = \frac{1}{\pi^2} \int_0^\pi \cos(x) \cos(y) + \sin(x) \sin(y) dx dy = \frac{2}{\pi^2}.
\]

Finally, given an orthonormal \( U \) of size \( d \times d \), \( d \geq 4 \), we use (22) and (25) to bound

\[
\mathbb{E}\left[ \left\| U - \prod_{k=1}^{d/2} G_{ik,jk} \right\|_F^2 \right] = 2d - 2 \sum_{k=1}^{d/2} \mathbb{E}[\| U_{ik,jk} \|_*] \leq 2d - \pi \sum_{k=1}^{d/2} \mathbb{E}[\text{tr}(U_{ik,jk})] \]

\[
\leq 2d - \pi \mathbb{E}[\text{tr}(U)] = 2d - \pi \mathbb{E}\left[ \sum_{t=1}^{d} |U_{tt}| \right] = 2d - \sqrt{2\pi d},
\]

(26)

where we have used that \( \mathbb{E}\left[ \sum_{t=1}^{d} |U_{tt}| \right] = \sqrt{2\pi} d^{-1/2} \) because the diagonal elements of \( U \) can be viewed as Gaussian random variables with zero mean and standard deviation \( d^{-1/2} \) (as the columns of \( U \) are normalized in the \( \ell_2 \) norm) \( \text{[Jiang(2006)]} \) and because the \( \ell_1 \) norm of a standard Gaussian random vector of size \( d \) is \( \sqrt{2\pi} d^{-1/2} \).

In (22) we could use the expected value calculated in (35) but we reach a worse, lower, constant in (26) for the \( -\sqrt{d} \) term and therefore a worse overall bound. 

**Proof of Theorem 3.** Given the orthonormal \( U \), by \( \text{[Golub & Van Loan(1996)]}[\text{Theorem 5.2.1]} \), we can construct its QR factorization using a set of Givens rotations \( \text{[Golub & Van Loan(1996)]}[\text{Chapter 5.2.5]} \). After introducing zeros in the first \( r \) columns of \( U \), by left multiplication with Givens rotations, we reach its following partial triangularization

\[
J_{i_g,j_0} \cdots J_{i_1,j_1} U = \begin{bmatrix}
D'' & 0_{r \times (d-r)} \\
0_{(d-r) \times r} & U'
\end{bmatrix},
\]

(27)
where the diagonal matrix $D''$ of size $r \times r$ has entries $D''_{tt} \in \{\pm 1\}$ and $U'$ of size $(d-r) \times (d-r)$ is orthonormal. To introduce the zeros on the $t$th column we need $(d-t)$ Givens rotations and therefore to bring $U$ to the structure in (27) we need $g = \frac{r}{2}(2d-r-1)$ Givens rotations which we have denoted $J_{t}^{t}, k = 1, \ldots, g$. We are exploiting the fact that the triangularization of an orthogonal matrix leads to a $\pm 1$ diagonal. Then we might consider a good approximation to $U$ the product $\hat{U} = J_{t}^{T} \ldots J_{g}^{T} D$, where $D = \begin{bmatrix} D'' & 0_{(d-r) \times r} \\ 0_{(d-r) \times r} & D' \end{bmatrix}$ with $D'_{tt} = \text{sgn}(U'_{tt})$ and $D''$ is taken from (27). The goal of the diagonal matrix $D$ is to ensure that the product in $\hat{U}$ has a nonnegative diagonal. Then, given $g$ transforms we can bound

$$
\| U - J_{t}^{T} \ldots J_{g}^{T} D \|_F^2 = 2(d - |r|) - 2tr(D'U').
$$

(28)

If we consider $\tilde{G}_{ij}$ in (2) instead of the rotations $J_{t}^{T}$ then the quantity on the right becomes an upper bound, since Givens rotations are a special case of $\tilde{G}_{ij}$ – we can always initialize the $G_{i,j,k}$ of Algorithm 1 with the $J_{t}^{T}$ defined above and the iterative procedure is guaranteed not to worsen the factorization. Therefore, the result follows after using $E(\text{tr}(D'U')) = E \left[ \sum_{t=1}^{d-|r|} |U'_{tt}| \right] = \sqrt{2(d - |r|)}\pi^{-T}$. 

**Proof of Theorem 4.** First, we introduce the off-diagonal “norm”, i.e., the square-root of the squared sum of the off-diagonal elements of an orthonormal matrix $U \in \mathbb{R}^{d \times d}$ as

$$
\text{off}(U)^2 = \sum_{t=1}^{d} \sum_{q=1, q\neq t}^{d} U_{tq}^2 = \| U \|_F^2 - \sum_{t=1}^{d} U_{tt}^2 = d - \sum_{t=1}^{d} U_{tt}^2.
$$

(29)

Better approximations $\hat{U}$ of $U$ lead to lower off$(U\hat{U}^T)$, as $U\hat{U}^T$ approaches the identity. If we use this measure, we reach the following result.

We use the fact that $C_{ij}$ is added to the diagonal of $U$, but only to $U_{ii}$ and $U_{jj}$. The quantity $f(\gamma) = (U_{ii} + \gamma C_{ij})^2 + (U_{jj} + (1 - \gamma) C_{ij})^2, \gamma \in \mathbb{R}$, is minimized for $C_{ij} \neq 0$ when $\gamma_0 = \frac{1}{2} + \frac{U_{ij} - U_{ii}}{2C_{ij}}$ (and therefore $f(\gamma_0) = \frac{1}{2}\| U_{\{i,j\}} \|_F^2$) which leads to

$$
\text{off}(UG_{ij}^T)^2 = d - \sum_{t=1, t \notin \{i,j\}}^{d} U_{tt}^2 - f(\gamma) \leq d - \sum_{t=1}^{d} U_{tt}^2 - f(\gamma_0)
$$

$$
= d - \sum_{t=1}^{d} U_{tt}^2 + U_{ii}^2 + U_{jj}^2 - f(\gamma_0) = \text{off}(U)^2 + \frac{(U_{ii} - U_{jj})^2}{2} - C_{ij}(U_{ii} + U_{jj}) - \frac{C_{ij}^2}{2}
$$

(30)

$$
= \text{off}(U)^2 + \frac{(U_{ii} - U_{jj})^2}{2} - \| U_{\{i,j\}} \|_F^2 - (U_{ii} + U_{jj})^2 = \text{off}(U)^2 + U_{ii}^2 + U_{jj}^2 - \| U_{\{i,j\}} \|_F^2.
$$

We now use the explicit formulas for the singular values of a $2 \times 2$ matrix and the fact that

$$
\| U_{\{i,j\}} \|_F^2 = s_1^2 + s_2^2 + 2s_1s_2 = \| U_{\{i,j\}} \|_F^2 + 2|\text{det}(U_{\{i,j\}})|,
$$

(31)

and expand this expression to get in (30)

if $\text{det}(U_{\{i,j\}}) \geq 0$ : \hspace{1em} \text{off}(UG_{ij}^T)^2 \leq \text{off}(U)^2 + \frac{(U_{ii} - U_{jj})^2 - (U_{ij} - U_{ji})^2}{2},$

if $\text{det}(U_{\{i,j\}}) < 0$ : \hspace{1em} \text{off}(UG_{ij}^T)^2 \leq \text{off}(U)^2 + \frac{(U_{ii} + U_{jj})^2 - (U_{ij} + U_{ji})^2}{2}.$
Nuclear norms

\[ P(X = x) \]

Un-normalized scores \( C_{ij} \)

\[ P(X = C_{ij}) \]

\[ u \]

\[ C_{ij}(u) \]

\[ (1 - u)^2 \]

Empirical mean

Therefore, to guarantee \( \text{off}(UG_{ij}^T)^2 \leq \text{off}(U)^2 \) we need \( 2(U_{ii}^2 + U_{jj}^2) \leq \|U_{\{i,j\}}\|^2_2 \) which is equivalent to

\[
\begin{align*}
\text{if } \text{det}(U_{\{i,j\}}) &\geq 0 : \quad (U_{ii} - U_{jj})^2 \leq (U_{ij} - U_{ji})^2, \\
\text{if } \text{det}(U_{\{i,j\}}) &< 0 : \quad (U_{ii} + U_{jj})^2 \leq (U_{ij} + U_{ji})^2.
\end{align*}
\]

(32)

In this paper we assume that \( U \) is taken randomly from the Haar measure \footnote{Johansson(1997)} and then modified to have positive diagonal. Therefore, we have \( U_{tt} \geq 0 \) for all \( t \) by construction, otherwise we would just consider the update \( U_{tt} \leftarrow \text{sign}(U_{tt})U_{tt} \). Moreover, as the algorithm progresses we continue to have that \( \text{det}(U_{\{i,j\}}) \geq 0 \) because each \( G_{ij} \) adds a positive amount (the \( C_{ij} \) value) to the diagonal elements \( U_{ii} \) and \( U_{jj} \) thus converging towards \( I_{d \times d} \) in the sense of \footnote{Jiang(2006)}.

In a similar way we can construct a lower bound. Assuming w.l.o.g. that \( U_{ii} \geq U_{jj} \geq 0 \), the quantity \( f(\gamma) = (U_{ii} + \gamma C_{ij})^2 + (U_{jj} + (1 - \gamma)C_{ij})^2 \) is maximized when \( \gamma_0 = 1 \) and therefore \( f(\gamma_0) = (U_{ii} + C_{ij})^2 + U_{jj}^2 \) which, similarly to \footnote{Jiang(2006)}, leads to

\[
\text{off}(UG_{ij}^T)^2 \geq \text{off}(U)^2 - C_{ij}(2U_{ii} + C_{ij}).
\]

(33)

**More on Remark 4.** Understanding the properties of these \( C_{ij} \) is of crucial importance for our approach. First, notice the effect one generalized Givens transformation has: we have \( \|U - G_{ij}\|_F^2 = \|UG_{ij}^T - I\|_F^2 = 2d - 2\text{tr}(UG_{ij}^T) \), which together with \footnote{Jiang(2006)} leads to

\[
\text{tr}(UG_{ij}^T) = \text{tr}(U) + C_{ij} \leq d.
\]

(34)

In this case, the \( G_{ij} \) “pushes” \( UG_{ij}^T \) towards the identity matrix by “contributing” \( C_{ij} \) to the diagonal of \( U \), i.e., we are estimating the inverse of \( U \) which in this case is just the transpose.

Notice that \( 0 \leq C_{ij} \leq 4 \). The minimum is achieved for symmetric positive semidefinite matrices (because in this case the eigenvalues and singular values are the same and therefore the nuclear norm equals the trace) and the maximum for \( U_{\{i,j\}} = -I_{2 \times 2} \). This immediately leads to a local optimality condition for our approach: there is no \( G_{ij} \) to improve the approximation if all \( U_{\{i,j\}} \) are symmetric positive definite. Assume now we are given a random orthogonal matrix. Because the singular values \( s_{1,2} \) depend on the entries of \( U_{\{i,j\}} \) which we model as Gaussian random variables with zero mean and standard deviation \( d^{-1/2} \) \footnote{Jiang(2006)}, we have by a direct calculation that \( \mathbb{E}[s_1] \approx 1.7724d^{-1/2} \).
Figure 7: Empirical mean (left) and maximum (right) values of $C_{ij}$ for the toy matrix $U_{\{i,j\}}$ where the diagonal elements $U_{ii}$ and $U_{jj}$ (both in $[0, 1]$) are fixed and the off-diagonals entries denoted $z_1$ and $z_2$ are uniform random variables in the interval $[-\sqrt{1-\beta}, \sqrt{1-\beta}]$ where $\beta = \max(U_{ii}^2, U_{jj}^2)$ since the columns and rows of $U$ are $\ell_2$ normalized. Low values (close to 0) are coded as dark blue while high values (close to 2) are coded as dark red.

and $E[s_2] \approx 0.5190d^{-1/2}$ which leads to $E[\|U_{\{i,j\}}\|_*] \approx 2.2914d^{-1/2}$. The trace is summation of two absolute value Gaussian random variables and therefore $E[\text{tr}(U_{\{i,j\}})] = 2\sqrt{2(\pi d)^{-1}}$ which leads to

$$E[C_{ij}] \approx 0.6956d^{-1/2}. \Box$$

More on Remark 5. To see how the scores $C_{ij}$ depend on the diagonal entries of our toy model, by direct calculation we have that

$$E[C_{ij}(u)] = \frac{1}{2\pi \text{erf}^2\left(\frac{1}{\sqrt{1-u^2}}\right) \int \int \sqrt{1-u^2} \exp\left(\frac{-z_1^2 + z_2^2}{2}\right) C_{ij}(u) \, dz_1 \, dz_2 \approx (1 - u)^2. \quad (36)$$

We show in Figure 6 the empirical results (mean and standard deviation of $C_{ij}$) on the toy matrix $U_{\{i,j\}} = \begin{bmatrix} u & z_2 \\ z_1 & u \end{bmatrix}$ for $0 < u < 1$. The empirical mean follows the approximation in Remark 5 (and is tight for $u \leq 0.7$) while we notice that the variance is high for almost the whole interval. In Figure 7 we show the average (left) and maximum (right) costs $C_{ij}$ achieved for another toy model where the diagonal elements are distinct $U_{\{i,j\}} = \begin{bmatrix} U_{ii} & z_2 \\ z_1 & U_{jj} \end{bmatrix}$ for $0 \leq U_{ii}, U_{jj} \leq 1$.

Finally, notice that when $U_{\{i,j\}} = \begin{bmatrix} u & U_{ij} \\ U_{ij} & u \end{bmatrix}$ we have $C_{ij} = 2(U_{ij} - u)$ if $u \leq U_{ij}$ and zero otherwise, and when $U_{\{i,j\}} = \begin{bmatrix} u & -U_{ij} \\ U_{ij} & u \end{bmatrix}$ we have $C_{ij} = 2\sqrt{u^2 + U_{ij}^2} - 2u$ indicating that skew symmetric sub-matrices have higher $C_{ij}$ than symmetric ones, in general. \Box