Maple Transactions

Rational Orthogonal Polynomials: applications and semi-dense matrices

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Abstract. Rational orthogonal matrices have many useful applications. Two contributions are presented here. There is a question whether a rational matrix can be reduced to QR factors which are also rational, and in particular whether the well known Householder method needs only rational arithmetic at each stage of its application. The conditions under which this is true are given. There have been several databases of rational orthogonal matrices proposed, which can be accessed by users. The matrices contained in the databases are dense, in the sense that there are no zero elements in the matrices. Here we describe the generation of semi-dense matrices, meaning that they are not sparse in the usual sense, but they do contain zero elements. If used for pedagogical purposes, such matrices can be used to provide simpler examples.

Additional Key Words and Phrases: Orthogonal matrices, Pythagorean vectors, Householder reflections

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1 Introduction

We define a *column-orthogonal* matrix Θ as one having the property $\Theta^T\Theta = D$, where D is a diagonal matrix with real entries. For such a matrix $\Theta\Theta^T$ is not necessarily diagonal. A *row-orthogonal* matrix Θ is one for which $\Theta\Theta^T = D$, while $\Theta^T\Theta$ is not necessarily diagonal. An orthogonal matrix obeys $\Theta^T\Theta = \Theta\Theta^T = d^2 I$, where d is a real scalar and I is the identity. If $d = 1$ then the matrix is orthonormal.

Rational orthogonal matrices are intrinsically related to Pythagorean n-tuples, because in order to normalize a rational vector of dimension n, some parts of its elements must form a Pythagorean n-tuple. Therefore we define a Pythagorean vector of dimension n as an integer vector with an integer norm. Such a vector can contain negative integers and zeros (unlike a Pythagorean n-tuple), but the absolute values of the non-zero elements form the elements of some Pythagorean m-tuple.

In various pedagogical applications, rational orthogonal matrices are beneficial. An obvious application is the teaching or testing of the orthogonalization of the basis of a subspace, or equivalently computing a QR decomposition. Current textbooks and exams frequently contain problems whose completion forces computations with square roots that do not simplify [2].

In order for instructors to take advantage of rational orthogonal matrices, they must have ways of obtaining them. This could be either by using software such as Maple to run programs that can generate them [1], or by access to a table of matrices. At present, there are tables available at

https://orcca.on.ca/files/OrthonormalMatrices/

We address here two questions. First, suppose a matrix A is created by the process of (1) choosing a matrix Q from a repository of rational orthogonal matrices; (2) generating a random upper triangular rational matrix R; (3) forming the product $A = QR$. Now ask that Householder transformations be used on A to obtain the Q, and R factors. The question is whether all of the intermediate steps will require only rational arithmetic. This is not obvious, since the householder process shrinks

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the working matrices by one dimension each step, and n-dimensional Pythagorean vectors are replaced by $(n-1)$-dimension vectors.
The second question concerns the generation of rational orthogonal matrices. The existing collections are dense, in the sense that every element is nonzero. Is it possible to mix 4-dimensional vectors and 3-dimensional vectors and create semi-dense matrices, in the sense that there are several zeros in the matrices?

2 Householder transformations

Householder transformations are taught in courses on *numerical* linear algebra, rather than introductory courses. A typical exercise runs as follows. Find the QR factors of the matrix

$$T = \begin{bmatrix} 1 & 4 & 3 \\ 4 & 1 & 2 \\ 3 & 2 & 1 \end{bmatrix}. \tag{1}$$

Using the first column as the vector z above: $z = [1, 4, 3]$ and then

$$v = \begin{bmatrix} ||z|| \\ 0 \\ 0 \end{bmatrix} - z = \begin{bmatrix} \sqrt{26} - 1 \\ -4 \\ -3 \end{bmatrix}. \tag{2}$$

The Householder matrix $H_1 = I - 2vv^T/(v^T v)$ is

$$H_1 = \begin{bmatrix} 1 - \dfrac{2(\sqrt{26}-1)^2}{25 + (\sqrt{26}-1)^2} & \dfrac{8(\sqrt{26}-1)}{25 + (\sqrt{26}-1)^2} & \dfrac{6(\sqrt{26}-1)}{25 + (\sqrt{26}-1)^2} \\ \dfrac{8(\sqrt{26}-1)}{25 + (\sqrt{26}-1)^2} & 1 - \dfrac{32}{25 + (\sqrt{26}-1)^2} & \dfrac{-24}{25 + (\sqrt{26}-1)^2} \\ \dfrac{6(\sqrt{26}-1)}{25 + (\sqrt{26}-1)^2} & \dfrac{-24}{25 + (\sqrt{26}-1)^2} & 1 - \dfrac{18}{25 + (\sqrt{26}-1)^2} \end{bmatrix}.$$

Simplifying the $(1, 1)$ element gives

$$1 - \frac{2(\sqrt{26}-1)^2}{25 + (\sqrt{26}-1)^2} = \frac{\sqrt{26}-1}{26 - \sqrt{26}} = \frac{\sqrt{26}}{26}. \tag{3}$$

This simplification task invites student error. In order to prevent squareroots from occurring, a matrix is constructed using a known Q and an R.

$$A = \frac{1}{9} \begin{bmatrix} 1 & 8 & -4 \\ 4 & -4 & -7 \\ 8 & 1 & 4 \end{bmatrix} \begin{bmatrix} 9 & 1 & 20/9 \\ 0 & 1 & -2/9 \\ 0 & 0 & 1/9 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 0 \\ 4 & 0 & 1 \\ 8 & 1 & 2 \end{bmatrix}. \tag{4}$$

The householder matrix H_1 is then

$$H_1 = \frac{1}{9} \begin{bmatrix} 1 & 4 & 8 \\ 4 & 7 & -4 \\ 8 & -4 & 1 \end{bmatrix}. \tag{5}$$

Householder matrices are rational when based on an integer vector v, which requires a Pythagorean z.
The Householder method next builds a matrix for the 2×2 submatrix. Thus from the Pythagorean vectors of dimension 3, a Pythagorean vector of dimension 2 is needed.

THEOREM 1. *Let $v_1 = [x_1, ..., x_n]$ and $v_2 = [y_1, ..., y_n]$ be Pythagorean. Let v_1 be orthogonal to v_2. Then the $(n-1)$-dimensional vector*

$$w = (X - x_1)[y2, ..., y_n] + y_1[x_2, ..., x_n],$$

where $X = ||v_1||$ and $Y = ||v_2||$ is Pythagorean and $||w||= (||v_1||-x_1)||v_2||$.

Proof:

$$\begin{aligned} ||w||^2 &= \sum_{k=2}^{n}[(X - x_1)y_k + y_1 x_k]^2 \\ &= (X - x_1)[XY^2 - x_1 Y^2]. \end{aligned}$$

This theorem underpins the statement that all intermediate expressions are rational.

3 Generating a database

The above approach assumes the existence of a database resource. The existing database contains matrices such as

$$\frac{1}{15}\begin{bmatrix} 3 & 6 & 6 & 12 \\ 6 & -13 & 2 & 4 \\ 6 & 2 & -13 & 4 \\ 12 & 4 & 4 & -7 \end{bmatrix}.$$

By taking out a common denominator, the matrix is presented as an integer matrix. Patterns in the elements are more easily noticed among integers. We call some a matrix ‘dense’, and the question arises whether matrices exist which are ‘semidense’, although not really sparse. One such matrix is

$$\frac{1}{15}\begin{bmatrix} 5 & 10 & 0 & 10 \\ 6 & 3 & 4 & -6 \\ 8 & 4 & -3 & -8 \\ 10 & -10 & 0 & 5 \end{bmatrix}.$$

$$\begin{bmatrix} 1 & 4 & 8 & 4 \\ 4 & 7 & -4 & 16 \\ 8 & -4 & 1 & 32 \\ 12 & 0 & 0 & -27 \end{bmatrix}\begin{bmatrix} 15 & 0 & 0 & 0 \\ 0 & 9 & 0 & 0 \\ 0 & 0 & 9 & 0 \\ 0 & 0 & 0 & 45 \end{bmatrix}^{-1}$$

In the last case, the matrix is orthonormal when multiplied out.

References

[1] A. C. Camargos Couto and D. J. Jeffrey. Maple makes manageable matrices. In J. Gerhard & I. Kotsireas, editor, *Third Maple Conference, MC 2019*, volume 1125 of *Communications in computer and information science*, pages 220–229. Springer, 2019.

[2] N. Khattak and D. J. Jeffrey. Rational orthonormal matrices. In T. Jebelean and V. Negru, editors, *SYNASC 2017*, pages 71–74. IEEE, 2017.

A Research Methods

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