Orthogonalization of Graded Sets of Vectors

I A SHRESHEVSKII

Institute for Physics of Microstructures, Russian Academy of Sciences
46 Uljanova street, Nizhnii Novgorod, RU-603600, Russia
E-mail: ilya@ipm.sci-nnov.ru

Received September 16, 2000; Accepted October 18, 2000

Abstract

I propose an orthogonalization procedure preserving the grading of the initial graded set of linearly independent vectors. In particular, this procedure is applicable for orthonormalization of any countable set of polynomials in several (finitely many) indeterminates.

There are two well-known procedures for orthogonalization of any set of linearly independent vectors in a linear space. The first of them boils down, essentially, to calculation of the \((-\frac{1}{2})\)-th power of the Gram matrix of the initial set (we refer to it as Gram method), and another one is the Gram–Schmidt process. The result of the Gram–Schmidt process essentially depends of the order of the elements in the set and the operations with Gram matrix seem to be impossible to perform in infinite dimensional spaces.

There are, however, some situations when one has to orthogonalize a finite or infinite set of linearly independent vectors in a linear space in such a way that the result would have some properties of the initial set. Observe that the set considered is not necessarily a basis. Any set consisting of linearly independent vectors will do. Observe also that I deal here with algebraic problems, no analytical problem (convergence, completeness, etc.) arises.

We consider some examples:

1. Let \( \{ e_m = e^{imx} \}_{m=-\infty}^{\infty} \) be a set of linearly independent vectors in \( L_2([0,2\pi],\rho) \), where \( \rho \) is any positive weight. If \( \rho \) is not constant, the elements of this set are not orthogonal, but have an important property \( e_m = \overline{e_{-m}} \), where the bar means complex conjugation. Is it possible to preserve this property under orthogonalization?

2. Let \( x = (x_1, \ldots, x_n) \), where \( x_i \in \mathbb{R} \), and \( m = (m_1, \ldots, m_n) \), where \( m_j \in \mathbb{Z}_+ \). Then the set \( \{ x^m : m \in \mathbb{Z}_+^n \} \), where \( x^m = x_1^{m_1} \cdots x_n^{m_n} \), is, due to Stone–Weierstrass theorem, a basis in \( L_2(\Omega) \) for a “good” bounded domain \( \Omega \subset \mathbb{R}^n \). This basis has no natural order, but has a natural grading: the degree of \( x^m \) is equal to \( |m| = m_1 + \cdots + m_n \). How to orthogonalize this basis and preserve the natural grading? Is this possible?
It is very strange that a very simple and natural answer to these and similar questions seems to be unknown. For this reason I present here the orthogonalization procedure, which combines some features of the Gram method and Gram–Schmidt process (in particular, it can be applied in infinite dimensional case) and gives a solution to the above problems and similar ones. Note in this connection that, although the orthogonalization problem is more than hundred years old, various aspects of the problem arise from time to time in connection with very interesting practical problems, see, e.g., [4].

Let \( \{ e_\alpha^k : \alpha \in I_k, k \in \mathbb{Z}_+ \} \) be a set of linearly independent vectors in a Hilbert space. We assume that all index sets \( I_k \) are finite. Let us inductively define the sets of vectors \( \{ f_\alpha^k : \alpha \in I_k \} \) by the formula

\[
f_\alpha^k = \sum_{\beta \in I_k} Q^k_{\beta \alpha} e_\beta^k + \sum_{j=0}^{k-1} \sum_{\beta \in I_j} P^k_{j \alpha} f_\beta^j,
\]

where the unknown matrices \( Q^k \) and \( P^k_{j \alpha} \) are determined from the orthonormality conditions for the system \( f^k \):

\[
\begin{align*}
(f_\alpha^k, f_\beta^k) &= \delta_{\alpha \beta}, \quad \alpha, \beta \in I_k, \\
(f_\alpha^k, f_\beta^j) &= 0, \quad \alpha \in I_k, \quad \beta \in I_j, \quad j \neq k.
\end{align*}
\]

Note, first of all, that the system \( f^k \) is linearly independent if and only if the matrices \( Q^k \) are nondegenerate. We will use this fact later.

From the last line in (2) and the definition (1) one immediately deduces that

\[
P^k_{j \alpha} = -\sum_{\gamma \in I_k} D^k_{j \gamma} Q^k_{\gamma \alpha},
\]

where we define the matrix \( D^k_{j \gamma} \) to be \( (e_\gamma^k, f_\beta^j) \). Let us substitute this expression for \( P \) in terms of \( Q \) and \( D \) into the first line in (3). We obtain, after simplification, a matrix equation of the form

\[
Q^k \Gamma^k Q^k = E,
\]

where \( B^k = \Gamma^k - \sum_{j=0}^{k-1} \Delta^k_j \) and \( \Gamma^k \) is the Gram matrix of the system \( \{ e_\alpha^k \}_{\alpha \in I_k} \) and \( E \) is the unit matrix.

Note that the matrix \( B \) is the Gram matrix for the linearly independent system of vectors in the Hilbert space

\[
h_\alpha^k = e_\alpha^k - \sum_{j=0}^{k-1} \sum_{\beta \in I_j} (e_\alpha^k, f_\beta^j) f_\beta^j.
\]

Hence, \( B^k \) is positive definite. So one can write the unique positive definite solution of the equation (4) in the “Gram” form

\[
Q^k = \left( \Gamma^k - \sum_{j=0}^{k-1} \Delta^k_j \right)^{-1/2}.
\]
This completes the orthonormalization process.

We consider now some simple examples.

3. If for all \( k \) the sets \( I_k \) are one-element sets, then the process described is exactly the Gram–Schmidt one.

4. In the above procedure \( \mathbb{Z}_+ \) can be replaced with any its finite subset. If such subset is a one-element set, then our process is exactly the Gram method.

These two examples show that the process suggested is simply a combination of two well-known processes.

5. Let \( I_0 = \{0\} \) and \( I_k = \{+,-\} \) for nonzero \( k \)'s. Let further \( e^k_\alpha \in L_2([0,2\pi], \rho) \) and 
\[ e^0 = 1, \quad e^k_{\pm} = e^{\pm imx}. \] (This is Example 1.) Then, clearly, \( f^0 = \text{const} \in \mathbb{R} \). Let us show now that if \( f^j_+ = f^j_- \) for all \( j < k \), then the same is true for \( k \) also.

Indeed, due to relations (2) and (3) we obtain

\[
\begin{align*}
f^k_{\pm} &= Q^k_{\pm+} \left(e^k_+ - \left(e^k_+, f^0_0\right) f^0_0\right) - \sum_{j=1}^{k-1} \left(\left(e^k_+, f^j_+\right)f^j_+ + \left(e^k_+, f^j_-\right)f^j_-\right) \\
&\quad + Q^k_{\pm-} \left(e^k_- - \left(e^k_-, f^0_0\right) f^0_0\right) - \sum_{j=1}^{k-1} \left(\left(e^k_-, f^j_+\right)f^j_+ + \left(e^k_-, f^j_-\right)f^j_-\right).
\end{align*}
\]

Now using inductive hypothesis and the fact that \( Q \) are Hermitean matrices, i.e., \( Q_{++}, Q_{+-} \in \mathbb{R} \) and \( Q_{++} = Q_{+-}^* \), it is easy to see that the vectors \( f^k_{\pm} \) are complex conjugate.

So we have obtained a simple affirmative answer to the question in Example 1.

It is interesting whether or not the above construction can be generalized to the vector systems in pseudo-euclidean spaces? Two problems arise in this case:

1) What shall we do with “isotropic” vectors?

2) For which matrix in the right hand side instead of the identity one, is equation (4) solvable?

Note in this connection that the Gram–Schmidt orthogonalization process is not applicable in the pseudo-euclidean case because even if the initial vector system does not contain isotropic vectors, such vectors can appear under execution of the process and terminate it.

We consider an example: if vector \( e_1 \) is isotropic, there does not exist any number \( \alpha \) such that vector \( e_1 + \alpha e_2 \) is pseudo-orthogonal to \( e_1 \) (of course, unless \( e_1 \) and \( e_2 \) are initially orthogonal).

Certain properties of bases and linear independent systems in pseudo-euclidean spaces are discussed in [1, 2]. In particular, Bognár proposes a “forceful” method for generalization of Gram–Schmidt process to pseudo-euclidean case for linearly ordered systems of vectors [3]. We use something like his method for graded systems.

In what follows we suppose that the pseudo-euclidean scalar product is “nondegenerate”, i.e., for any linearly independent finite system of vectors consisting of more than one element its Gram matrix is nondegenerate. In other words, this means that the
dimension of any maximal isotropic subspace (all of whose vectors are isotropic) does not exceed 1. Then any finite system of vectors, excluding one-element ones, may be “pseudo-orthonormalized” in the sense that the pseudo-norm, or “length”, of each final vector will be equal to \( \pm 1 \).

To this end, it suffices to determine the signature \((p, q)\) of the Gram matrix \(\Gamma\) of the initial system of vectors and then solve the equation

\[
R^\top \Gamma R = E_p \oplus (-E_q)
\]

for unknown matrix \(R\). If we write the Hermitean matrix \(\Gamma\) in the form \(\Gamma = U \Lambda U^\dagger\), where \(U\) is a unitary matrix and \(\Lambda = \Lambda_p \oplus (-\Lambda_q)\) is a diagonal matrix with \(p\) positive and \(q\) negative elements, then the solution of \((6)\) can be written in the form \(R = U \left( \Lambda_p^{-1/2} \oplus (-\Lambda_q^{-1/2}) \right)\).

Therefore, it is clear that the only trouble which might appear when dealing with graded systems of vectors in pseudo-euclidean spaces is when after the \(k\)-th step the set \(\{ f_k^\alpha : \alpha \in I_k \}\) consists of exactly one isotropic vector. There does not exist any general natural way to resolve this situation and details depend on the concrete case. A most simple idea is to include such a vector into the next, \((k + 1)\)-th, level set of vectors and then continue the process. This trick slightly violates the initial grading, but preserves the filtration.

The problems discussed stem from several sources. One is numerical analysis and data processing. Here the role of discrete Fourier transformation is well-known, but what should we do if our data is given on a nonuniform grid? For the answer see Example 1.

Another problem is orthonormalization of splines which constitute a not linearly ordered, but a graded set of functions.

D Leites and A Sergeev pointed out a totally different area in which the same question arises. These problems concern with new polynomials in several indeterminates connected with some Lie algebras and superalgebras and the space of these polynomials is naturally endowed with a nondegenerate indefinite metric, see [3]. For one indeterminate D Leites and A Sergeev can orthogonalize their polynomials; for several indeterminates these polynomials are not linearly ordered and they got stuck. By our method one can orthogonalize the polynomials in several indeterminates proposed in [3].

For the reader who wishes to compare various orthogonalization methods I suggest very transparent and user friendly paper by Srivastava [4].

Acknowledgements. I am thankful to D Leites and Stockholm University for hospitality, TBSS for financial support, and to T Ya Azizov for helpful comments.

References

[1] Bognár J, Indefinite Inner Product Spaces, Springer, Berlin–Heidelberg–NY, 1974.

[2] Gohberg I, Lancaster P and Rodman L, Matrices and Indefinite Scalar Products, Birkhäuser, Basel–Boston–Stuttgart, 1983.

[3] Leites D and Sergeev A, Orthogonal Polynomials of Discrete Variable and Lie Algebras of Complex Size Matrices, in Proceedings of M Saveliev Memorial Conference, MPI, Bonn, February, 1999, MPI-1999-36, 49–70; Teor. Mat. Fiz., 2000, V.123, N 2, 205–236 (Theor. Math. Phys., 2000, V.123, 582–609).
[4] Srivastava V, A Unified View of the Orthogonalization Methods. J. Phys. A: Math. Gen., 33 (2000), 6219–6222.