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# Numerical Gram–Schmidt orthonormalization

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## Abstract

A numerical Gram–Schmidt orthonormalization procedure is presented for constructing an orthonormal basis function set from a non-orthonormal set, when the number of basis functions is large. This method will provide a pedagogical illustration of the Gram–Schmidt procedure and can be presented in classes on numerical methods or computational physics.

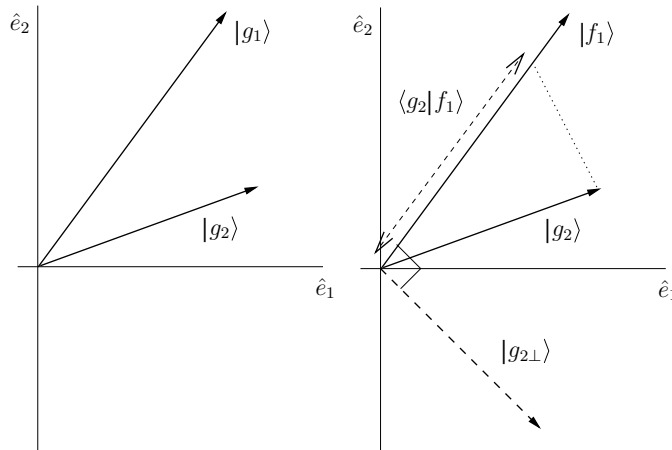
(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

The Gram–Schmidt orthonormalization method is typically introduced to junior and senior level undergraduate physics students as a way to construct a set of orthonormal basis functions from a set of non-orthonormal basis functions [1–3]. An orthonormal set makes computations in quantum mechanics much easier because the inner product takes on a simple form involving a Dirac delta function [3]. The Gram–Schmidt procedure is easily implemented when only a few orthonormal basis functions are needed, but numerical techniques are usually employed when a larger set of orthonormal basis functions is needed. However, these techniques are rarely taught in classes despite the practical advantages for solving many problems. We present the analytical and numerical approach of constructing orthonormal basis functions via the Gram–Schmidt procedure, and we discuss the limitations of the numerical approach.

The techniques presented here will provide students with a pedagogical example of how to implement the Gram–Schmidt procedure when the basis function set is large. It can be used in courses involving numerical methods or computational physics and is suitable for presentation to undergraduate physics, engineering and mathematics students.

Before discussing orthonormalization, we first establish some notation. Let  $\{|f_i\rangle\}$  be a set of column vectors and let  $\langle f_i| = |f_i\rangle^\dagger$ , where  $|f_i\rangle^\dagger$  is the complex conjugate and transpose of  $|f_i\rangle$ . The scalar product is defined as  $\langle f_i|f_j\rangle = \alpha$ , where  $\alpha$  is a real number. If the vectors  $|f_i\rangle$



**Figure 1.** Left: two normalized but non-orthogonal vectors,  $|g_1\rangle$  and  $|g_2\rangle$ . Right: an illustration of the Gram–Schmidt method, where a set of orthonormal basis vectors  $|f_i\rangle$  is constructed from a set of normalized but non-orthogonal basis vectors  $|g_i\rangle$ . After equating  $|g_1\rangle$  to  $|f_1\rangle$ ,  $|g_2\rangle$  is projected onto  $|f_1\rangle$  and the component parallel to  $|f_1\rangle$  is subtracted from  $|g_2\rangle$ , resulting in  $|g_{2\perp}\rangle$ . Finally,  $|g_{2\perp}\rangle$  is normalized to  $|f_2\rangle$ .

and  $|f_j\rangle$  satisfy  $\langle f_i | f_j \rangle = \delta_{ij}$ , then these vectors are said to be orthonormal and the set  $\{|f_i\rangle\}$  is an orthonormal set. In this paper, the vector notation can be written in function language as

$$\langle r | f_i \rangle = f_i(r)$$

and

$$\langle f_i | f_j \rangle = \int_0^\infty f_i^*(r) f_j(r) dr.$$

Therefore, in function language, orthonormality means

$$\int_0^\infty f_i^*(r) f_j(r) dr = \delta_{ij}.$$

We are interested in orthonormalizing a set of functions  $\{g_i(r)\}$  so that we obtain a new set  $\{f_i(r)\}$  which is orthonormal according to the conditions above.

## 2. The Gram–Schmidt method

The Gram–Schmidt method is used to construct an orthonormal set of basis vectors  $|f_i\rangle$  from a set of non-orthogonal but normalized basis vectors  $|g_i\rangle$ . The method is best illustrated graphically as in figure 1. In this figure, two arbitrarily positioned vectors  $|g_1\rangle$  and  $|g_2\rangle$  are chosen, which are normalized but not orthogonal.  $|g_1\rangle$  is chosen and set equal to  $|f_1\rangle$ . We will construct vectors orthogonal to the new normalized basis vector  $|f_1\rangle$ . First, we construct another vector  $|f_2\rangle$  which is orthogonal to  $|f_1\rangle$ . To do this, we use the vectors  $|f_1\rangle$  and  $|g_2\rangle$ . We project  $\langle g_2 |$  onto  $|f_1\rangle$  giving the component of  $|g_2\rangle$  that is parallel to  $|f_1\rangle$ . Now subtract from  $|g_2\rangle$  the parallel component  $\langle g_2 | f_1 \rangle |f_1\rangle$  along the  $|f_1\rangle$  direction giving

$$|g_{2\perp}\rangle = |g_2\rangle - \langle g_2 | f_1 \rangle |f_1\rangle.$$

Label this orthogonal vector as  $|g_{2\perp}\rangle$  since it is the component of  $|g_2\rangle$  perpendicular to  $|f_1\rangle$ , as seen in figure 1. Now that a vector orthogonal to  $|f_1\rangle$  has been constructed, the next step is to find the normalization constant  $N_2$  such that  $|f_2\rangle = N_2|g_{2\perp}\rangle$ :

$$|f_2\rangle = N_2(|g_2\rangle - \langle g_2|f_1\rangle|f_1\rangle).$$

The normalization condition is  $\langle f_2|f_2\rangle = 1$ , so that

$$\begin{aligned} N_2^2(\langle g_2| - \langle f_1|g_2\rangle\langle f_1|)(|g_2\rangle - \langle g_2|f_1\rangle|f_1\rangle) &= 1, \\ N_2^2(1 - \langle f_1|g_2\rangle^2) &= 1. \end{aligned}$$

Thus, the normalization constant is

$$N_2 = \sqrt{\frac{1}{1 - \langle f_1|g_2\rangle^2}}.$$

Now construct a vector orthonormal to both  $|f_1\rangle$  and  $|f_2\rangle$  by using the same procedure:

$$|f_3\rangle = N_3[|g_3\rangle - \langle f_2|g_3\rangle|f_2\rangle - \langle f_1|g_3\rangle|f_1\rangle],$$

where

$$N_3 = \frac{1}{\sqrt{1 - \langle f_2|g_3\rangle^2 - \langle f_1|g_3\rangle^2}}.$$

In general, we may construct a set of orthonormal basis  $|f_n\rangle$  from a set of normalized but non-orthogonal basis  $|g_n\rangle$  by using

$$|f_n\rangle = N_n \left[ |g_n\rangle - \sum_{i=1}^{n-1} t_{in} |f_i\rangle \right], \tag{1}$$

where

$$N_n = \sqrt{\frac{1}{1 - \sum_{i=1}^{n-1} t_{in}^2}}, \tag{2}$$

and

$$t_{in} = \langle f_i | g_n \rangle.$$

### 3. Analytical approach

Now we switch to basis functions in Hilbert space [3], for the purpose of illustrating the technique in quantum mechanics. As an example, we will construct an orthonormal basis  $f_i(r)$  from the non-orthogonal but normalized functions. Next consider a three-dimensional bound state problem. The reduced wavefunction must satisfy the boundary conditions. The boundary conditions are that the reduced wavefunction vanishes at  $r = 0$  and  $r = \infty$ . The Gaussian function in the next equation is an example of a function that satisfies the radial part of the three-dimensional bound state problem since it vanishes at  $r = 0$  and  $r = \infty$ , thus satisfying the boundary conditions for the reduced wavefunction:

$$g_i(r) = N_i^g r e^{-a_i r^2}, \tag{3}$$

where the normalization factor is obtained by requiring that

$$\int_0^\infty g_i^*(r) g_i(r) dr = 1,$$

thereby giving

$$N_i^g = \sqrt{\frac{4(2a_i)^{\frac{3}{2}}}{\sqrt{\pi}}}, \quad (4)$$

where  $a_i$  is a constant which is later taken to be  $i^2$  where  $i = 1, 2, 3, \dots$  when the numerical calculations are implemented. Projecting  $\langle r |$  onto equation (2),

$$f_2(r) = N_2[g_2(r) - t_{21}f_1(r)]. \quad (5)$$

The initial basis is chosen as  $f_1(r) = g_1(r)$ . Thus,

$$f_1(r) = N_1^g r e^{-a_1 r^2}. \quad (6)$$

From equations (5), (6) and (3) write

$$f_2(r) = N_2(N_2^g r e^{-a_2 r^2} - t_{21}N_1^g r e^{-a_1 r^2}), \quad (7)$$

where

$$t_{21} = \int_0^\infty g_2(r)f_1(r) dr = N_2^g N_1^g \int_0^\infty r^2 e^{-(a_1+a_2)r^2} dr.$$

Use the normalization conditions to obtain

$$\begin{aligned} t_{21} &= \sqrt{\frac{4(2a_2)^{\frac{3}{2}}}{\sqrt{\pi}}} \sqrt{\frac{4(2a_1)^{\frac{3}{2}}}{\sqrt{\pi}}} \int_0^\infty r^2 e^{-(a_1+a_2)r^2} dr \\ &= \sqrt{\frac{4(2a_2)^{\frac{3}{2}}}{\sqrt{\pi}}} \sqrt{\frac{4(2a_1)^{\frac{3}{2}}}{\sqrt{\pi}}} \frac{\sqrt{\pi}}{4(a_1+a_2)^{\frac{3}{2}}} = \frac{(4a_1a_2)^{\frac{3}{4}}}{(a_1+a_2)^{\frac{3}{2}}}. \end{aligned} \quad (8)$$

Now verify that the basis vectors are indeed orthonormal. Begin by showing that  $\langle f_1 | f_1 \rangle = 1$ :

$$\langle f_1 | f_1 \rangle = (N_1^g)^2 \int_0^\infty r^2 e^{-2a_1 r^2} = \frac{4(2a_1)^{\frac{3}{2}}}{\sqrt{\pi}} \frac{\sqrt{\pi}}{4(2a_1)^{\frac{3}{2}}} = 1.$$

Next, show that  $\langle f_2 | f_2 \rangle = 1$ , via

$$\begin{aligned} \langle f_2 | f_2 \rangle &= N_2^2 (N_2^g)^2 \int_0^\infty r^2 e^{-2a_2 r^2} dr + t_{21}^2 N_2^2 (N_1^g)^2 \int_0^\infty r^2 e^{-2a_1 r^2} dr \\ &\quad - 2N_2^2 N_2^g N_1^g t_{21} \int_0^\infty r^2 e^{-(a_1+a_2)r^2} dr. \end{aligned}$$

Evaluating the integrals and using the normalization conditions gives

$$\begin{aligned} \langle f_2 | f_2 \rangle &= \frac{4N_2^2 (2a_2)^{\frac{3}{2}}}{\sqrt{\pi}} \frac{\sqrt{\pi}}{4(2a_2)^{\frac{3}{2}}} + \frac{4N_2^2 (2a_1)^{\frac{3}{2}}}{\sqrt{\pi}} \frac{\sqrt{\pi}}{4(2a_1)^{\frac{3}{2}}} \\ &\quad - 2N_2^2 t_{21} \sqrt{\frac{4(2a_2)^{\frac{3}{2}}}{\sqrt{\pi}}} \sqrt{\frac{4(2a_1)^{\frac{3}{2}}}{\sqrt{\pi}}} \frac{\sqrt{\pi}}{4(a_1+a_2)^{\frac{3}{2}}}. \end{aligned}$$

Simplifying and using equation (8),

$$\langle f_2 | f_2 \rangle = N_2^2 [1 - t_{21}^2] = \frac{1 - t_{21}^2}{1 - t_{21}^2} = 1.$$

The last step is to verify the orthogonality of  $|f_1\rangle$  and  $|f_2\rangle$ . Thus,

$$\langle f_1 | f_2 \rangle = N_1^g N_2 \left[ N_2^g \int_0^\infty r^2 e^{-(a_1+a_2)r^2} dr - N_1^g t_{21} \int_0^\infty r^2 e^{-2a_1 r^2} dr \right] = 0.$$

As we have seen, constructing and verifying the orthonormal basis analytically can be time consuming. We now devise a numerical scheme for generating the orthonormal basis and use numerical integration to verify orthonormality.

#### 4. Computational approach

We will construct the orthonormal basis functions  $f_i(r)$  using the non-orthogonal but normalized functions  $g_i(r)$ . We have shown that the orthonormal basis may be expressed in equation (1) as

$$|f_n\rangle = N_n \left[ |g_n\rangle - \sum_{i=1}^{n-1} t_{in} |f_i\rangle \right], \quad (9)$$

where

$$t_{in} = \langle f_i | g_n \rangle = \int_0^\infty f_i(r) g_n(r) \, dr,$$

and the normalization is given by equation (2). As can be seen in equation (1),  $t_{in}$  should be computed before generating the orthonormal basis. Projecting  $\langle g_j |$  onto equation (1) gives

$$\langle g_j | f_n \rangle = N_n \left[ \langle g_j | g_n \rangle - \sum_{i=1}^{n-1} t_{in} \langle g_j | f_i \rangle \right].$$

We define  $G_{jn} \equiv \langle g_j | g_n \rangle$  and project with  $\langle g_j |$  onto equation (1) to obtain the recursive relation

$$t_{jn} = N_n \left[ G_{jn} - \sum_{i=1}^{n-1} t_{in} t_{ij} \right], \quad (10)$$

where  $j > n > i$ . An expression for  $G_{jn}$  is

$$G_{jn} = N_j^g N_n^g \frac{\sqrt{\pi}}{4(a_j + a_n)^{\frac{3}{2}}},$$

where the normalization constants are given by equation (4). We note that since the functions  $g(r)$  and  $f(r)$  are real,  $t_{in} = t_{ni}$  and  $G_{in} = G_{ni}$ . As described in the analytical approach,  $|f_1\rangle = |g_1\rangle$ . Next, we calculate the elements in which  $t_{j1} = G_{j1}$ . Then, a general  $t_{jn}$  is calculated from equation (10) by iteration.

We can construct a matrix from the inner product of the orthonormalized basis functions,

$$D = \begin{pmatrix} \langle f_1 | f_1 \rangle & \langle f_1 | f_2 \rangle & \cdots & \langle f_1 | f_m \rangle \\ \langle f_2 | f_1 \rangle & \langle f_2 | f_2 \rangle & \cdots & \langle f_2 | f_m \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle f_m | f_1 \rangle & \langle f_m | f_2 \rangle & \cdots & \langle f_m | f_m \rangle \end{pmatrix} \quad (11)$$

where  $m$  is the total number of orthonormal basis functions. Since the matrix elements of  $D$  are  $\langle f_i | f_j \rangle$ ,

$$\langle f_i | f_j \rangle = \int_0^\infty f_i(r) f_j(r) \, dr.$$

If  $|f_i\rangle$  and  $|f_j\rangle$  are indeed orthonormal, then  $D$  should be the identity matrix. However, in practice,  $D$  will deviate from the identity matrix when a large number of functions are used. The reason for this is that orthogonality comes from the cancellation of the oscillatory features from the functions. As we increase the number of functions, the numerical cancellations of the functional oscillations become inaccurate because of the limitations of machine precision.

The deviation of the  $D$  matrix from the identity matrix depends on  $m$ .

The orthonormal basis functions were constructed numerically, and thus the *analytical* functional forms of all of the orthonormal basis functions are not required. The advantage of the numerical approach is that the student does not have to manipulate the cumbersome analytical functional forms. Since the basis functions were constructed numerically, one can compute the matrix elements of  $D$  and verify the orthonormality of  $\langle f_i | f_j \rangle$  using a numerical integration method known as Gaussian quadrature [1, 4], which is now discussed for completeness.

## 5. Gaussian quadrature

Gaussian quadrature [1, 4] is a useful computational tool used to perform numerical integration. It approximates an integral using the following relation:

$$\int_{-1}^1 f(x) dx \approx \sum_{i=0}^{n-1} w_i f(x_i), \quad (12)$$

where  $f$  is the function,  $x_i$  are the roots of the Legendre polynomials,  $n$  is the number of Gaussian points (number of roots of the Legendre polynomial), and  $w_i$  are the weights determined from the derivatives of the Legendre polynomials  $P'_i(x_i)$  evaluated at  $x_i$ . The weights are determined using

$$w_i = \frac{2}{(1 - x_i^2)[P'_i(x_i)]^2}.$$

The limits of the integrals must be transformed such that equation (12) is satisfied. This can be done with a suitable substitution of the variable. If one has an integral of the form  $\int_0^\infty f(x') dx'$ , the following transformation may be used before implementing Gaussian quadrature:

$$x' = \tan \left[ \frac{\pi}{4} (x + 1) \right].$$

Using the above substitution,  $x' \rightarrow 0$  as  $x \rightarrow -1$  and  $x' \rightarrow \infty$  as  $x \rightarrow 1$  gives

$$\begin{aligned} \int_0^\infty f(x') dx' &= \int_{-1}^1 f \left\{ \tan \left[ \frac{\pi}{4} (x + 1) \right] \right\} \frac{\pi}{4} \sec^2 \left[ \frac{\pi}{4} (x + 1) \right] dx \\ &\approx \sum_{i=0}^{n-1} f \left\{ \tan \left[ \frac{\pi}{4} (x_i + 1) \right] \right\} \frac{\pi}{4} w_i \sec^2 \left[ \frac{\pi}{4} (x_i + 1) \right]. \end{aligned}$$

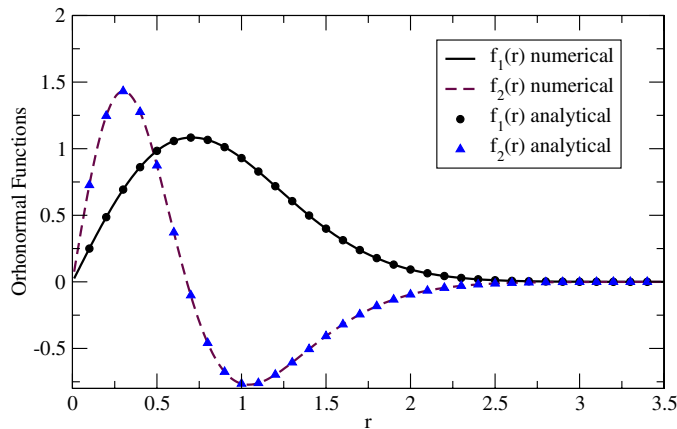
After this transformation, Gaussian quadrature is applied to evaluate the integral.

## 6. Results

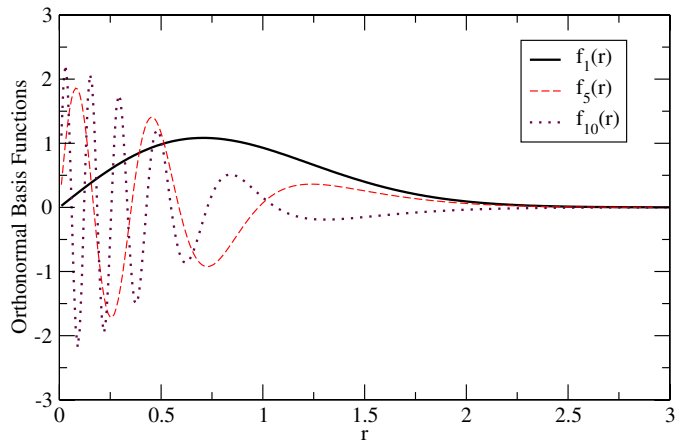
In figure 2, we have plotted the first two orthonormal basis functions,  $f_1(r)$  and  $f_2(r)$ , generated from the non-orthonormal basis functions defined in equation (3). The solid and dashed lines represent the orthonormal functions calculated numerically with the Gram–Schmidt method, and the circles and triangles represent the functions generated analytically as in equations (6) and (7). The analytical results are in excellent agreement with numerical results.

Next, in figure 3, we have plotted the  $i$ th orthonormalized basis function, where  $i = 1, 5$  and 10. The numerical procedure is advantageous because the student will be able to obtain many orthonormalized functions without having to calculate each orthonormal function analytically. It would be a very time consuming task to calculate ten orthonormal functions





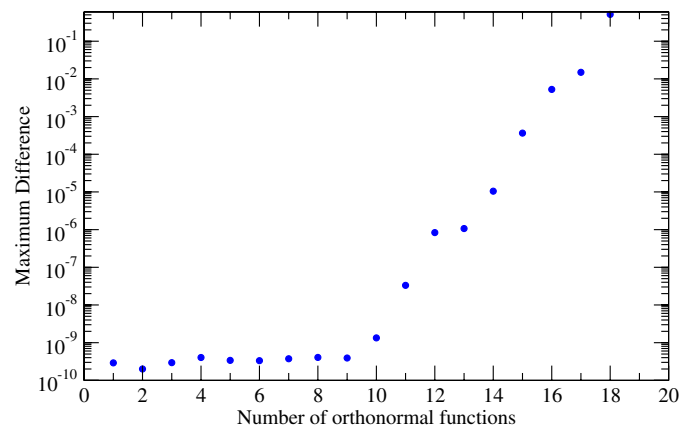
**Figure 2.** The first two orthonormal basis functions  $f_1(r)$  and  $f_2(r)$  are plotted. The solid and dashed lines represent the numerically calculated orthonormal functions generated by the Gram–Schmidt method. The circles and triangles represent the analytically calculated orthonormal functions.



**Figure 3.** A plot of three orthonormal basis functions. Each orthonormal function is generated numerically using the Gram–Schmidt method.

analytically. This method proves to be efficient and is simple enough to be included in an introductory quantum mechanics course.

Although the numerical approach is simple and efficient, students should be aware of its limitations. If we construct a matrix  $D$  from the inner product of orthonormal basis vectors, as in equation (11), and compare it with the identity matrix, we may identify the limitations of the numerical approach. In figure 4, we have plotted the maximum difference between the  $D$  matrix and the identity matrix with respect to the size of the  $D$  matrix. Note that the deviation of  $D$  from the identity matrix is negligible for matrix sizes of  $10 \times 10$  or smaller. Afterwards the deviation increases more quickly for larger matrix sizes, as explained in section 4.



**Figure 4.** The maximum difference between the  $D$  matrix and the identity matrix with respect to the size of the  $D$  matrix.

## 7. Conclusions

The Gram–Schmidt orthonormalization procedure has been applied to a set of non-orthogonal basis functions and a numerical scheme was devised. This scheme will be useful when the set of basis functions is large. The method can be used as a numerical assignment in quantum mechanics classes. It can also be used in numerical analysis or computational physics courses as a numerical example of a technique that is widely used in physics, engineering and mathematics. Students will gain experience in Gram–Schmidt orthonormalization, Hilbert space methods, Gaussian integration and general numerical techniques.

## Acknowledgment

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