1. Introduction

In the fields of computer science, engineering, biology, chemistry, statistics and many others, having a strong background in mathematics has always been necessary. As we continue to explore the components of the world in which we live, the link between mathematics and the sciences is becoming more apparent and more important to understand. With the availability of high speed computing, entire new fields such as computational biology have emerged. Linear algebra is being utilized extensively to linearize problems that have no exact mathematical solution so that computers can solve them. Linear algebra is a branch of mathematics based on the ideas of vectors and matrices, as well as the study of linear transformations and of systems of linear equations. Biologists want to be able to express a biological event or situation in terms of a mathematical model that can be simulated through the use of a high-speed computer program. By finding a linear approximation of an event we wish to model (linearization), we can use the tools for working with linear systems to analyze the model. The synergistic relationship between the disciplines of mathematics, biology and computer science has been drawn together as a single field appropriately named computational biology (also called bioinformatics).

Using mathematical techniques to model population dynamics began in the 19th century with the advent of the Lotka-Volterra predator-prey equations. Mathematical biology models a variety of biological processes such as the mechanics of tissues, the interaction of cell populations, kinetics of enzymes, swarm behavior, carcinogenesis, cancer simulation, and many others [1] by using various mathematical techniques.
The field of biomolecular modeling, or the study of the structure and function of molecules, began relatively recently, in the 1960’s. Its origins come from molecular mechanics. The idea behind molecular mechanics is that molecules can be represented as a mechanical system; thus we can calculate a molecule’s geometry and various other properties from experimental data. In 1946, Frank Westheimer recorded the first successful attempts at molecular mechanics calculations in his work on racemization rates [2].

In the 1960’s, researchers in Georgia, Israel, Michigan and New York independently began to study systematic force fields and developed parameters for families of chemical compounds [3, p. 7]. They compared the experimental observations of structure to their calculated results. However, it wasn’t until the 1980’s and the arrival of the super-computers that the field began to grow rapidly. Great gains in technology and modeling techniques followed, and in 1990 the Human Genome Project (HGP) began[4].

The HGP is an international effort that has 20 sequencing centers in six countries: China, England, France, Germany, Japan, and the United States [5]. The project aimed to discover and make accessible all the estimated 30-40,000 human genes. As part of the HGP, additional parallel studies have helped to develop advanced technologies for interpreting the functions of the human genes found and catalogued.

The two experimental techniques that are used most extensively to determine information on the structure of protein molecules are X-ray diffraction (also called X-ray crystallography) and NMR (nuclear magnetic resonance.) Although the results from
X-ray crystallography are more detailed than NMR, the well-ordered crystals needed for crystallography are difficult to grow. Also, amplitude, wavelength and phase are needed in order to infer the atoms’ positions from X-ray crystallography and the phase is not obtainable from the X-ray experiments. The phase can be calculated from the other data, but the mathematical analysis limits the amount of accurate data obtainable [3, p. 16]. This is called the phase-problem in crystallography. Though less detailed, NMR is more versatile than X-ray diffraction in that it gives structural as well as dynamic information. NMR produces a system of distances between hydrogen atoms within a small distance from each other. Because the molecules being studied are so large, both the NMR and X-ray diffraction measurement methods require the use of today’s super-computers to interpret the resulting data and produce the molecular structure.

The applications of molecular modeling are many and varied. They range from drug design and cosmeceuticals, to designer foods and materials. The structure of molecules is tied closely to their function, so being able to produce drugs with specific structural compositions leads to their acting in a specific role, such as competing with viruses for the receptor sites on cells thus limiting infection. The AIDS drugs that have been developed work on this principle. Another successful drug developed using molecular modeling is a thrombin inhibitor that is used to treat and manage clotting-related diseases [3, p. 53].

Designer, genetically modified foods have met a great deal of public resistance in the supermarkets both here and abroad. There is great fear that they will be disastrous for the environment. However, altering the gene structure of a plant does not necessarily mean that the goal is to produce huge or more prolific produce. There are goals to
produce plants with edible vaccines against Hepatitis B, or develop bacteria that produce human insulin [3, p. 56]. There have also been some less than successful gene structure manipulations in plants. One such flop was the Flavr Savr tomato; it looked (and stayed) beautiful as it had been modified to have less ripening enzyme, but was considered a disappointment by consumers because it had very little flavor [3, p.57].

Computational methods are important in all these developments as they allow the screening and optimizing of the designer molecules involved. Advancements in the experimental techniques for gleaning the data and the computer capabilities and mathematical algorithms used in analysis of the data continue to move computational biology ahead by leaps and bounds.

This fascinating topic of molecular modeling relies heavily on the tools of linear algebra to enable the study of the structure and function of bio-molecules. By representing information as an ordered list of components (a vector) we can condense and manipulate the data with relative ease. Since the information available is the distances between atoms in a molecule, and since what is desired is the molecular structure, which can be precisely described by coordinates of the atoms, it is important to be able to compute one from the other. This type of problem is called the “Distance Geometry Problem”; the solution uses linear algebra to recreate the structure of molecules, such as proteins, from ‘known’ distances that are either measured directly (X-ray diffraction or NMR) or are expected from the nature of the atoms of the molecule.

In this particular discussion of the structure of a molecule, we assume it is a rigid configuration. In other words, the atoms in the molecule keep the same distances relative
to the other atoms while their locations in 3-space may change. The structure of the molecule is not affected by rotation or translation.

The association of the coordinates in 3-space of a set of atoms to the distances between pairs of atoms is fairly straightforward, and most high school geometry students are capable of evaluating the distances. Sophisticated techniques can be used to solve the non-trivial problem of computing coordinates from distances.

The distance between points A and B can be found by setting up a right triangle configuration and using the Pythagorean Formula:

\[
(a_1 - b_1)^2 + (a_2 - b_2)^2 = d(A, B)^2 \quad (1)
\]

However, as simple as this approach is to use going from the coordinates of the points to the distances between them, the computation that allows us to go in reverse—given the distances between points, find their coordinates—is much less trivial.

By introducing some new and powerful tools from linear algebra, we will be able to calculate and manipulate our distance data efficiently and thereby determine a set of points to describe the structure. These resultant points represent a configuration congruent (through translation, rotation, or reflection) to our original structure.

2. Linear Algebra Background

The basic linear algebra terms and computations that will be used are defined in this section. These terms include the definition of a vector and vector space; the dot
product; norm; eigenvalues and eigenvectors; orthogonal, orthonormal, and independent vectors; basis and span.

We begin now with the idea of a vector being an ordered list of values. A vector is visualized with an arrow whose tail is at the origin and whose head is located at the point whose coordinates correspond to the vector’s values. In this paper, our discussion revolves around atoms in 3-space and so a vector that describes an atom’s position in relation to the origin will be a list of three numbers representing the \( x \), \( y \) and \( z \) coordinates of the atom. However, abstract vectors can have any size, \( \mathbf{v} = [v_1, v_2, \ldots, v_n] \) with each \( v_i \) corresponding to a specific characteristic or coordinate.

The \( n \)-dimensional real vector space, \( \mathbb{R}^n \), is the set of \( n \)-tuples of real numbers (i.e. vectors) with coordinate-wise addition and multiplication of a vector by a real number (scalar).

The set of all linear combinations of the set of vectors in \( V = \{ \mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n \} \) is called their \textit{span}. We can represent the span of \( V \) by \( \text{span}(\mathbf{v}_1, \ldots, \mathbf{v}_n) = \{ c_1 \mathbf{v}_1 + c_2 \mathbf{v}_2 + \ldots + c_n \mathbf{v}_n : c_i \) are arbitrary real numbers\}. The vectors \( \mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n \) are \textit{linearly independent} if and only if the only solution to \( c_1 \mathbf{v}_1 + c_2 \mathbf{v}_2 + \ldots + c_n \mathbf{v}_n = 0 \) is the trivial one, \( c_1 = c_2 = \ldots = c_n = 0 \)

\textbf{Example 1:} Let \( \mathbf{v}_1 = [1,2,0] \), \( \mathbf{v}_2 = [-1,1,2] \), \( \mathbf{v}_3 = [3,0,-4] \).

\[
\begin{bmatrix}
 1 & -1 & 3 & 0 \\
 2 & 1 & 0 & 0 \\
 0 & -2 & -4 & 0
\end{bmatrix}
\]

This vector equation can be represented by a matrix equation:

\[
\begin{bmatrix}
 1 & -1 & 3 & c_1 \\
 2 & 1 & 0 & c_2 \\
 0 & 2 & -4 & c_3
\end{bmatrix}
\begin{bmatrix}
 0 \\
 0 \\
 0
\end{bmatrix}
\]
This, in turn, can be solved by reduction using reduced row echelon form (RREF).

\[
\begin{bmatrix}
1 & -1 & 3 \\
2 & 1 & 0 \\
0 & 2 & -4
\end{bmatrix} \rightarrow
\begin{bmatrix}
1 & -1 & 3 \\
0 & 3 & -6 \\
0 & 2 & -4
\end{bmatrix} \rightarrow
\begin{bmatrix}
1 & -1 & 3 \\
0 & 1 & -2 \\
0 & 0 & 0
\end{bmatrix}
\]

thus:

\[
\begin{bmatrix}
1 & 0 & 1 \\
0 & 1 & -2 \\
0 & 0 & 1
\end{bmatrix}
\]

This is equivalent to the system:

\[
\begin{align*}
\begin{bmatrix}
c_1 \\
c_2 \\
c_3
\end{bmatrix} &= \\
1\begin{bmatrix}c_1 \\
c_2 \\
c_3
\end{bmatrix} &= 0 \\
0\begin{bmatrix}c_1 \\
c_2 \\
c_3
\end{bmatrix} &= 0 \\
0\begin{bmatrix}c_1 \\
c_2 \\
c_3
\end{bmatrix} &= 0
\end{align*}
\]

so we see that \(c_1, c_2, c_3\) need not be zero for the second relation equation to equal zero. In particular, \(c_1 = -1, c_2 = 2, c_3 = 1\) is a solution. Therefore, \(v_1, v_2, v_3\) are not linearly independent.

**Example 2:** Let \(v_1 = [1,2,0], v_2 = [0,-1,1], v_3 = [1,2,-1]\)

\[
\begin{bmatrix}
1 & 0 & 1 \mid c_1 \\
2 & -1 & 2 \mid c_2 \\
0 & 1 & -1 \mid c_3
\end{bmatrix}
\]

\[
\begin{bmatrix}
1 & 0 & 1 \mid c_1 \\
2 & -1 & 2 \mid c_2 \\
0 & 1 & -1 \mid c_3
\end{bmatrix}
\rightarrow
\begin{bmatrix}
1 & 0 & 1 \mid c_1 \\
0 & -1 & 0 \mid c_2 \\
0 & 0 & -1 \mid c_3
\end{bmatrix}
\rightarrow
\begin{bmatrix}
1 & 0 & 0 \mid c_1 \\
0 & 1 & 0 \mid c_2 \\
0 & 0 & 1 \mid c_3
\end{bmatrix}
\]

It is clear at this point that \(c_1 = 0, c_2 = 0, c_3 = 0\) is the only solution. Thus \(v_1, v_2, v_3\) are linearly independent.

If vectors \(w_1, w_2, \ldots, w_n\) are in \(\mathbb{R}^n\) and they are linearly independent and are a spanning set for \(\mathbb{R}^n\), then they form a basis of \(\mathbb{R}^n\).
A set of \( n \) vectors of order \( k \) can be combined in a matrix with dimensions \( n \times k \).

\[
\begin{bmatrix}
  x_{11} & x_{12} & \cdots & x_{1k} \\
  x_{21} & x_{22} & \cdots & x_{2k} \\
  \vdots & \vdots & \ddots & \vdots \\
  x_{n1} & x_{n2} & \cdots & x_{nk}
\end{bmatrix}
\]

The vectors for a set of points in 3-space can be organized in a matrix such that each row is the coordinate vector information for one atom, i.e. a 3-vector. If a structure has 4 atoms, the matrix will have 4 rows (the atoms) and 3 columns (their coordinates) making it a \( 4 \times 3 \) matrix.

**Example 3:** Let vectors for the original locations of the four atoms be:

\[
\begin{align*}
\mathbf{a}_1 &= [0, 2, 3], \\
\mathbf{a}_2 &= [-5, 1, 0], \\
\mathbf{a}_3 &= [7, -5, 3], \\
\mathbf{a}_4 &= [-2, 4, -1],
\end{align*}
\]

then the matrix is

\[
A^o = \begin{bmatrix}
  0 & 2 & 3 \\
  -5 & 1 & 0 \\
  7 & -5 & 3 \\
  -2 & 4 & -1
\end{bmatrix}
\]

where \( A^o \) signifies the original vectors (the original locations). We can never determine the matrix \( A^o \) from distance only, since translation affects \( A^o \) but not distances. What we determine in our distance geometry problem is a matrix of atom positions that represent the same structure as \( A^o \). We can translate \( A^o \) in order for its last atom to be located at the origin as an ‘anchor.’

\[
A^o + T = A \quad (\text{where } T \text{ is the translation matrix})
\]

\[
A^o + T = \begin{bmatrix}
  0 & 2 & 3 \\
  -5 & 1 & 0 \\
  7 & -5 & 3 \\
  -2 & 4 & -1
\end{bmatrix} + \begin{bmatrix}
  2 & -4 & 1 \\
  2 & -4 & 1 \\
  2 & -4 & 1 \\
  2 & -4 & 1
\end{bmatrix} = \begin{bmatrix}
  2 & -2 & 4 \\
  -3 & -3 & 1 \\
  9 & -9 & 4 \\
  0 & 0 & 0
\end{bmatrix} = A
\]
The dot product (also called the scalar product or inner product) of two vectors is simply the sum of the product of their corresponding elements. The dot product is commutative, because if \( x = [x_1, x_2, ..., x_n] \) and \( y = [y_1, y_2, ..., y_n] \), then the dot product of \( x \) and \( y \) is:

\[
x \cdot y = x_1y_1 + x_2y_2 + \ldots + x_ny_n = y_1x_1 + y_2x_2 + \ldots + y_nx_n = y \cdot x
\]

Another useful result from a dot product is that \( x \cdot y = 0 \) if and only if the vectors are orthogonal (or perpendicular). Technically, in \( \mathbb{R}^n \) this is the definition of perpendicular, but it coincides with our intuition in \( \mathbb{R}^2 \) and \( \mathbb{R}^3 \).

**Example 4:** Let \( x = [2, 2, 0] \) and \( y = [3, -3, 0] \), we know that the vectors lie in the \( x-y \) plane and we can see that \( x \) is on a 45º angle from the \( x \)-axis and \( y \) is on a -45º angle from the \( x \)-axis. Thus the angle between them is 90º and they are perpendicular.

Now, if we find the dot product of the vectors we see that it equals zero, thus they are perpendicular:

\[
x \cdot y = 2(3) + 2(-3) + 0(0) = 0
\]

When we take a dot product of a vector with itself, we get a result that begins to resemble the distance formula from (1). If \( x = [x_1, x_2, ..., x_n] \), then
\[ \mathbf{x} \cdot \mathbf{x} = x_1^2 + x_2^2 + \ldots + x_n^2 = \sqrt{x_1^2 + x_2^2 + \ldots + x_n^2} \]

If we take the square root of this expression, we get the distance between the end point (head) and the initial point (tail) of a vector when its tail is at the origin.

\[ \sqrt{\mathbf{x} \cdot \mathbf{x}} = \sqrt{x_1^2 + x_2^2 + \ldots + x_n^2} = \sqrt{(x_1 - 0)^2 + (x_2 - 0)^2 + \ldots + (x_n - 0)^2} \]

**Example 5:** Let \( \mathbf{x} = [3,1,-2] \), then the dot product is \( \mathbf{x} \cdot \mathbf{x} = 3^2 + 1^2 + (-2)^2 = 14 \), and the length of vector \( \mathbf{x} \) is \( \sqrt{\mathbf{x} \cdot \mathbf{x}} = \sqrt{14} \).

In linear algebra, the length is called the norm. The norm of \( \mathbf{x} \) is written as \( ||\mathbf{x}|| \) and is defined to be the square root of the dot product of \( \mathbf{x} \) with itself:

\[ ||\mathbf{x}|| = \sqrt{\mathbf{x} \cdot \mathbf{x}} = \text{length of } \mathbf{x} = \sqrt{x_1^2 + x_2^2 + \ldots + x_n^2} \]

We saw previously that the distance between two points, \( A = (a_1,a_2,a_3) \) and \( B = (b_1,b_2,b_3) \), in 3-space is found thusly:

\[ d(A,B) = \sqrt{(a_1 - b_1)^2 + (a_2 - b_2)^2 + (a_3 - b_3)^2} \]

Thus we see that the norm of the difference, \( ||\mathbf{x} - \mathbf{y}|| \), is the distance between the endpoints of the two vectors, \( \mathbf{x} = [x_1, x_2, \ldots, x_n] \) and \( \mathbf{y} = [y_1, y_2, \ldots, y_n] \):

\[ ||\mathbf{x} - \mathbf{y}|| = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2 + \ldots + (x_n - y_n)^2} \]

To build a distance matrix \( D = [d_{i,j}] \) for a molecule with \( n \) atoms, we must calculate the distances between all combinations of the \( i \)th and \( j \)th atoms. The distance matrix of the \( n \) atoms whose coordinates are \( \mathbf{x}^{(0)}, \ldots, \mathbf{x}^{(n)} \) is defined to be:

\[ D = \begin{bmatrix}
  d_{1,1} & d_{1,2} & \cdots & d_{1,n} \\
  d_{2,1} & d_{2,2} & \cdots & d_{2,n} \\
  \vdots & \vdots & \ddots & \vdots \\
  d_{n,1} & d_{n,2} & \cdots & d_{n,n}
\end{bmatrix} \]

where \( d_{i,j} = ||\mathbf{x}^{(i)} - \mathbf{x}^{(j)}|| \).
Since the distance between an atom and itself is 0,

\[ D = \begin{bmatrix}
  0 & d_{1,2} & \cdots & d_{1,n} \\
  d_{2,1} & 0 & \cdots & d_{2,n} \\
  \vdots & \vdots & \ddots & \vdots \\
  d_{n,1} & d_{n,2} & \cdots & 0
\end{bmatrix} \]

As noted earlier, \( D \) is easy to compute from the coordinates of the atoms.

Example 6: Let there be 3 atoms in a molecule with coordinate vectors:

\[ \mathbf{v}_1 = \begin{bmatrix} 0 & 4 & -3 \end{bmatrix}, \mathbf{v}_2 = \begin{bmatrix} 2 & -2 & 2 \end{bmatrix}, \mathbf{v}_3 = \begin{bmatrix} 1 & 0 & -1 \end{bmatrix} \]

\[ d_{1,2} = \sqrt{(0-2)^2 + (4-(-2))^2 + (-3-2)^2} = \sqrt{4 + 36 + 25} = \sqrt{65} = d_{2,1} \]

\[ d_{1,3} = \sqrt{(0-1)^2 + (4-0)^2 + (-3-(-1))^2} = \sqrt{21} = d_{3,1} \]

\[ d_{2,3} = \sqrt{(2-1)^2 + ((-2)-0)^2 + (2-(-1))^2} = \sqrt{14} = d_{3,2} \]

\[ D = \begin{bmatrix}
  \sqrt{65} & \sqrt{21} \\
  \sqrt{21} & \sqrt{14} \\
  \sqrt{14} & 0
\end{bmatrix} \]

Eigenvalues and eigenvectors are important tools used in linear algebra and throughout the sciences. An eigenvector of a square matrix is a vector whose direction is preserved (or reversed) by matrix multiplication, although length may not be preserved.

If, for square matrix \( A \), there exists a non-zero vector \( \mathbf{v} \) such that \( A\mathbf{v} = \lambda \mathbf{v} \), where \( \lambda \) is a scalar (real or complex number), then \( \mathbf{v} \) is called an eigenvector that belongs to the eigenvalue \( \lambda \).\(^1\) Eigenvalues can be calculated from the characteristic polynomial of the matrix for small matrices. The equation \( p(x) = \det(xI - A) \) is called the characteristic polynomial.

\(^1\) Note: if \( \mathbf{v} \) is an eigenvector, so is \( c\mathbf{v} \) for any non-zero scalar, \( c \).
polynomial of matrix $A$. To find the eigenvalues of $A$, we solve the characteristic equation $p(\lambda) = 0$, i.e. find the roots of the characteristic polynomial. This gives eigenvalues because our definition of the relationship between eigenvectors and eigenvalues:

$$A \mathbf{v} = \lambda \mathbf{v}$$

$$\lambda \mathbf{v} - A \mathbf{v} = 0$$

$$(\lambda I - A)\mathbf{v} = 0$$

And there exists $\mathbf{v} \neq 0$ such that $(\lambda I - A)\mathbf{v} = 0$ if and only if $\det(\lambda I - A) = 0$.

**Example 7:** If $A = \begin{bmatrix} 2 & 3 \\ 1 & 4 \end{bmatrix}$ then the characteristic polynomial of $A$ is

$$p(x) = \det\begin{bmatrix} x & 0 \\ 0 & x \end{bmatrix} - \begin{bmatrix} 2 & 3 \\ 1 & 4 \end{bmatrix} = \det\begin{bmatrix} x - 2 & -3 \\ -1 & x - 4 \end{bmatrix} =$$

$$(x - 2)(x - 4) - (-1)(-3) = x^2 - 6x + 5$$

We set $p(\lambda) = 0$ and solve for the roots:

$$\lambda^2 - 6\lambda + 5 = 0$$

$$(\lambda - 5)(\lambda - 1) = 0$$

so the eigenvalues (roots) of $A$ are $\lambda = 5, 1$.

It is important to list the eigenvalues in decreasing order as it will make a difference later on in our problem solving. Once we have found the eigenvalues, we are ready to determine the eigenvector(s) that belong to each eigenvalue.

**Example 8:** We substitute in each eigenvalue and solve for the corresponding $\mathbf{v}$. 

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\( \lambda = 5: \begin{bmatrix} 5 & 0 \\ 0 & 5 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} v = 0 \)

\[
\begin{bmatrix} 3 \\ -1 \end{bmatrix} v_1 \\
\begin{bmatrix} -3 \\ 1 \end{bmatrix} v_2 = 0
\]

This system is solved by Gauss-Jordan elimination to find the reduced row echelon form (RREF).

\[
\text{RREF: } \begin{bmatrix} 1 \\ 0 \end{bmatrix} v_1 - \begin{bmatrix} 1 \\ 0 \end{bmatrix} v_2 = 0
\]

\( v_1 - v_2 = 0 \)

\( v_1 = v_2 \) and an eigenvector for \( \lambda = 5 \) is \( \begin{bmatrix} 1 \\ 1 \end{bmatrix} \).

\( \lambda = 1: \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} v = 0 \)

\[
\begin{bmatrix} -1 \\ -1 \end{bmatrix} v = 0
\]

\[
\text{RREF: } \begin{bmatrix} -1 \\ 0 \end{bmatrix} v_1 - \begin{bmatrix} -3 \\ 0 \end{bmatrix} v_2 = 0
\]

\( -v_1 - 3v_2 = 0 \)

\( v_1 = -3v_2 \) and an eigenvector for \( \lambda = 1 \) is \( \begin{bmatrix} -3 \\ 1 \end{bmatrix} \).

In the process of finding the coordinate matrix in the distance geometry problem, it is necessary to have an orthormal basis of eigenvectors. This is a basis of eigenvectors that are unit vectors (have length 1) and pair-wise orthogonal (dot product of any 2 vectors equals 0.) We can construct such a basis of eigenvectors using the Gram-Schmidt process. To normalize a non-zero vector \( v \) means to divide it by its length.
to obtain a unit vector, \( \frac{v}{\|v\|} \), in the same direction as \( v \). Given an independent set of vectors \( V = \{v_1, v_2, \ldots, v_n\} \), the Gram-Schmidt process produces an orthonormal set \( U = \{u_1, u_2, \ldots, u_n\} \) with the same span as \( V \) by creating an orthogonal set \( W = \{w_1, w_2, w_3, \ldots, w_n\} \) and then normalizing each \( w_i \) to a \( u_i \). This resulting orthonormal basis is \( U = \{u_1, u_2, u_3, \ldots, u_n\} \).

If \( V = v_1, v_2, v_3, \ldots, v_n \) is a basis for \( \mathbb{R}^n \), then we construct the orthogonal basis \( W = \{w_1, w_2, w_3, \ldots, w_n\} \) for \( \mathbb{R}^n \) as follows:

\[
\begin{align*}
  w_1 &= v_1 \\
  w_2 &= v_2 - \frac{\langle v_2, w_1 \rangle}{\langle w_1, w_1 \rangle} w_1, & \text{where } \langle a, b \rangle = a \cdot b \\
  w_3 &= v_3 - \frac{\langle v_3, w_1 \rangle}{\langle w_1, w_1 \rangle} w_1 - \frac{\langle v_3, w_2 \rangle}{\langle w_2, w_2 \rangle} w_2 \\
  & \quad \vdots \\
  w_n &= v_n - \frac{\langle v_n, w_1 \rangle}{\langle w_1, w_1 \rangle} w_1 - \frac{\langle v_n, w_2 \rangle}{\langle w_2, w_2 \rangle} w_2 - \cdots - \frac{\langle v_n, w_{n-1} \rangle}{\langle w_{n-1}, w_{n-1} \rangle} w_{n-1}
\end{align*}
\]

Now we normalize to get:

\[
  u_i = \frac{w_i}{\|w_i\|}
\]

Example 9: Let \( V = \{v_1, v_2, v_3\} \) where

\[
  v_1 = \begin{bmatrix} 1 \\ 2 \\ -1 \end{bmatrix}, \quad v_2 = \begin{bmatrix} 0 \\ 1 \\ -1 \end{bmatrix}, \quad v_3 = \begin{bmatrix} 3 \\ 7 \\ 1 \end{bmatrix}
\]

Then \( w_1 = \begin{bmatrix} 1 \\ 2 \\ -1 \end{bmatrix} \) and \( u_1 = \frac{1}{\sqrt{6}} \begin{bmatrix} 1 \\ 2 \\ -1 \end{bmatrix} \)
Thus the orthonormal basis for \( V \) is \( U = \{ u_1, u_2, u_3 \} \). The real \( n \times n \) matrix \( U \) is an orthogonal matrix if the columns of \( U \) are an orthonormal set of vectors, i.e. if \( U^T U = I \).

Note: This means \( U^T = U^{-1} \).

### 3. Real symmetric matrices.

We need several properties of real, symmetric matrices. The transpose \( A^T \) of a matrix \( A \) exchanges the rows and columns. The Hermitian adjoint of \( A \), \( A^* \), is the complex conjugate of the transpose of \( A \) (for real matrix, \( A^* = A^T \)). A matrix is symmetric if it is equal to its transpose. In general, a real matrix may have complex (nonreal) eigenvalues. This is not the case for a symmetric matrix, but to prove all eigenvalues of a symmetric matrix are real, we must consider the possibility of a complex eigenvalue and complex eigenvector.

**Lemma 1:** Let \( A \) be a real symmetric matrix. Every eigenvalue of \( A \) is real.

**Proof:** Let \( \lambda \) be an eigenvalue of \( A \) and \( \mathbf{v} \) be an eigenvector, i.e. \( A\mathbf{v} = \lambda \mathbf{v} \).

\[
\lambda (\mathbf{v}^* \mathbf{v}) = \mathbf{v}^* (A\mathbf{v}) = \mathbf{v}^* (Av) = (\mathbf{v}^* A)\mathbf{v} = (Av)^* \mathbf{v} = (\lambda \mathbf{v})^* \mathbf{v} = (\overline{\lambda}) \mathbf{v}^* \mathbf{v}.
\]

Since \( \mathbf{v} \neq 0 \) and \( \mathbf{v}^* \mathbf{v} \neq 0 \), and \( \lambda = \overline{\lambda} \), i.e. \( \lambda \) is real. ■

**Lemma 2:** If \( A \) is a real symmetric matrix with distinct eigenvalues \( \lambda \neq \mu \) with real eigenvectors \( \mathbf{v} \) and \( \mathbf{w} \) respectively, then \( \mathbf{v} \) and \( \mathbf{w} \) are orthogonal.
Proof: \[ v^T (Aw) = v^T (\mu w) = (\mu v)^T w = \mu (v \cdot w) \]
\[ v^T (Aw) = v^T A^T w = (Av)^T w = (\lambda v)^T w = \lambda (v \cdot w) \]

thus \( \mu (v \cdot w) = \lambda (v \cdot w) \), so \( (\mu - \lambda)(v \cdot w) = 0 \).

Since we assumed \( \lambda \neq \mu \), \( v \cdot w = 0 \).

Therefore, \( v \) and \( w \) are orthogonal. \( \blacksquare \)

**Lemma 3:** Let \( A \) be a real, symmetric, \( n \times n \) matrix, then \( A \) has a set of \( n \) independent eigenvectors [6, p. 443].

**Lemma 4:** Let \( A \) be a real, symmetric, \( n \times n \) matrix, then \( A \) has a basis of orthonormal eigenvectors.

**Proof:** By Lemma 3, \( A \) has a basis \( B \) of eigenvectors. By Lemma 2, eigenvectors for distinct eigenvalues are already orthogonal. If \( B \) contains more than one eigenvector for one eigenvalue \( \lambda \), apply the Gram-Schmidt process to the subset of \( B \) consisting of all the eigenvectors for eigenvalue \( \lambda \). Repeat for each eigenvalue having multiple eigenvectors to obtain an orthogonal basis of eigenvectors. Then normalize each vector. \( \blacksquare \)

The next theorem is easily derived from the previous lemmas.

**Theorem 1:** For any real symmetric matrix \( H \), there exists a real orthogonal matrix \( U \) such that \( U^T H U = \Sigma \), where \( \Sigma \) is a real diagonal matrix of the eigenvalues of \( H \). (The columns of \( U^T \) are the orthonormal eigenvectors of \( H \).)

**Proof:** By Lemma 4, \( H \) has an orthonormal basis of eigenvectors \([u^{(i)},...,u^{(n)}]\) for eigenvalues \( \lambda_1,...,\lambda_n \). Let \( U = [u^{(i)},...,u^{(n)}] \) and let \( \Sigma \) be the diagonal matrix with
diagonal elements $\lambda_1, \ldots, \lambda_n$. Then $U$ is orthogonal, so $U^T = U^{-1}$.

$$HU = [Hu^{(1)}, \ldots, Hu^{(n)}] = [\lambda_1 u^{(1)}, \ldots, \lambda_n u^{(n)}] = U\Sigma,$$ so $U^T HU = \Sigma$. □

In the decomposition $H = U\Sigma U^T$, the 0 eigenvalues and their eigenvectors do not affect the construction. That is, direct computation shows that we have the following result.

**Corollary 1:** If $\Sigma = \text{diag}(\lambda_1, \ldots, \lambda_k, 0, \ldots, 0)$, $U = [u^{(1)}, \ldots, u^{(n)}]$, and $H = U\Sigma U^T$ then

$$H = \tilde{U} \Sigma \tilde{U}^T$$ where $\tilde{U} = [u^{(1)}, \ldots, u^{(k)}]$, and $\tilde{\Sigma} = \text{diag}(\lambda_1, \ldots, \lambda_k)$.

The decomposition $H = \tilde{U} \Sigma \tilde{U}^T$ is called the (reduced) singular value decomposition (SVD) of $H$.

### 4. Distance Geometry Problem.

In the paper *Linear Algebra in Biomolecular Modeling* [7], the challenge of mapping from distances to coordinates (used in NMR structure determination) is presented and solved. This discussion is based on that paper.

In order to find coordinates, we must examine the relationship between distances and coordinates. Recall that $A^o$ denotes the $n \times 3$ matrix of coordinates of $n$ atoms and $A$ denotes the result of translating the $n$th atom to the origin. Let $b^{(0)} = [b_{i,3}, b_{i,2}, b_{i,1}]$.

$$i = 1 \ldots n - 1, \text{ where } A = \begin{bmatrix} b^{(1)} \\ \vdots \\ b^{(n-1)} \\ 0 \end{bmatrix} \text{ and } B = \begin{bmatrix} b^{(1)} \\ \vdots \\ b^{(n-1)} \end{bmatrix}. \text{ Then since } b^{(0)} \text{ is the difference in coordinates between the } i^{th} \text{ atom and the } n^{th} \text{ atom, } \|b^{(0)}\| = d_{in} \text{ and}$$
\[ d_{i,j} = \sqrt{(b_{i1} - b_{j1})^2 + (b_{i2} - b_{j2})^2 + (b_{i3} - b_{j3})^2} \]

\[ d_{i,j}^2 = (b_{i1}^2 - 2b_{i2}b_{j1} + b_{j1}^2) + (b_{i2}^2 - 2b_{i3}b_{j2} + b_{j2}^2) + (b_{i3}^2 - 2b_{i3}b_{j3} + b_{j3}^2) \]

\[ d_{i,j}^2 = (b_{i1} + b_{i2} + b_{i3})^2 + (b_{j1} + b_{j2} + b_{j3})^2 - 2(b_{i1}b_{j1} + b_{i2}b_{j2} + b_{i3}b_{j3}) \]

\[ d_{i,j}^2 = \|\mathbf{b}^{i}\|^2 + \|\mathbf{b}^{j}\|^2 - 2\mathbf{b}^{i} \cdot \mathbf{b}^{j} \]

\[ d_{i,j}^2 = d_{i,n}^2 + d_{j,n}^2 - 2\mathbf{b}^{i} \cdot \mathbf{b}^{j} \]

\[ \mathbf{b}^{i} \cdot \mathbf{b}^{j} = \frac{d_{i,n}^2 + d_{j,n}^2 - d_{i,j}^2}{2} \]

Define \( \hat{D} \) to be the \((n-1) \times (n-1)\) matrix whose \( ij^{th} \) entry (for \( i,j = 1,...,n-1 \)) is

\[ \hat{d}_{i,j} = \frac{d_{i,n}^2 + d_{j,n}^2 - d_{i,j}^2}{2} \]

where \( d_{i,j} \) is the distance between atom \( i \) and atom \( j \) from the distance matrix. Then we have proved

**Theorem 2:** \( \hat{D} = BB^T \).

**Example 10:** Let \( A^o = \begin{bmatrix} 3 & 1 & 0 \\ 2 & 3 & 2 \\ -1 & 1 & 1 \\ 7 & -2 & -2 \\ 2 & -1 & 1 \end{bmatrix} \), then \( A = \begin{bmatrix} 1 & 2 & -1 \\ 0 & 4 & 1 \\ -3 & 2 & 0 \\ 5 & -1 & -3 \\ 0 & 0 & 0 \end{bmatrix} \) and \( B = \begin{bmatrix} 1 & 2 & -1 \\ 0 & 4 & 1 \\ -3 & 2 & 0 \\ 5 & -1 & -3 \end{bmatrix} \). The distance matrix \( D = \begin{bmatrix} 0 & 3 & \sqrt{17} & \sqrt{29} & \sqrt{6} \\ \sqrt{17} & 0 & \sqrt{14} & \sqrt{66} & \sqrt{17} \\ \sqrt{29} & \sqrt{66} & 0 & \sqrt{82} & \sqrt{13} \\ \sqrt{6} & \sqrt{17} & \sqrt{13} & 0 & \sqrt{35} \end{bmatrix} \) so \( \hat{D} = \begin{bmatrix} 6 & 7 & 1 & 6 \\ 7 & 17 & 8 & -7 \\ 1 & 8 & 13 & -17 \\ 6 & -7 & -17 & 35 \end{bmatrix} \).

The entries are just computed from the formula.
\[ d_{1,1} = \frac{\sqrt{6^2} + \sqrt{6^2} - 0}{2} = 6 \]

eg.,

\[ d_{1,2} = \frac{\sqrt{6^2} + \sqrt{17^2} - 3^2}{2} = 7 = \frac{\sqrt{17^2} + \sqrt{6^2} - 3^2}{2} = d_{2,1} \]

It is also easy to verify by computation that \( B^T B = \hat{D} \).

There is a clever use of Theorem 1 to solve for the coordinate matrix we want:

\[
\begin{align*}
U^T \hat{D} U &= \Sigma \\
UU^T \hat{D} U &= U \Sigma U^T \\
\hat{D} &= U \Sigma U^T
\end{align*}
\]

Recall that \( \hat{D} = BB^T \), so all eigenvalues of \( \hat{D} \) are nonnegative. Since \( B = (n-1) \times 3 \), rank \( B \leq 3 \). Multiplication by another matrix cannot raise the rank, so \( \text{rank } \hat{D} \leq 3 \). That is, at most 3 of the eigenvalues of \( \hat{D} \) are nonzero. By Corollary 1 with \( k=3 \), \( \hat{D} = \tilde{U} \tilde{\Sigma} \tilde{U}^T \).

Remembering that \( \tilde{\Sigma} \) is a diagonal matrix of three nonnegative eigenvalues of \( \hat{D} \), we can take the principal square root of \( \tilde{\Sigma} \) to obtain \( B \):

\[
\hat{D} = \tilde{U} \sqrt{\tilde{\Sigma}} \sqrt{\tilde{\Sigma}}^{-T} \tilde{U}^T = \left( U \sqrt{\Sigma} \right) \left( U \sqrt{\Sigma} \right)^T
\]

Therefore, \( B' = \tilde{U} \sqrt{\tilde{\Sigma}} \) is a possible solution of the distance geometry problem. This solution is not unique, since the molecule can be rotated or reflected without changing distances.
Example 11: As in Example 10, let \( D = \begin{bmatrix} 0 & 3 & \sqrt{17} & \sqrt{29} & \sqrt{6} \\ 3 & 0 & \sqrt{14} & \sqrt{66} & \sqrt{17} \\ \sqrt{17} & \sqrt{14} & 0 & \sqrt{82} & \sqrt{13} \\ \sqrt{29} & \sqrt{66} & \sqrt{82} & 0 & \sqrt{35} \\ \sqrt{6} & \sqrt{17} & \sqrt{13} & \sqrt{35} & 0 \end{bmatrix} \) so

\[
\hat{D} = \begin{bmatrix} 6 & 7 & 1 & 6 \\ 7 & 17 & 8 & -7 \\ 1 & 8 & 13 & -17 \\ 6 & -7 & -17 & 35 \end{bmatrix}.
\]

The diagonal matrix of the eigenvalues of \( \hat{D} \) (excluding all 0 eigenvalues), denoted by \( \tilde{\Sigma} \), is:

\[
\begin{bmatrix}
47.6682 & 0 & 0 \\
0 & 20.3421 & 0 \\
0 & 0 & 2.98967
\end{bmatrix}
\]

so \( \sqrt{\tilde{\Sigma}}= \begin{bmatrix}
6.90422 & 0 & 0 \\
0 & 4.51022 & 0 \\
0 & 0 & 1.72907
\end{bmatrix} \).

The matrix of orthonormal eigenvectors for the nonzero eigenvalues of \( \hat{D} \) is \( \tilde{U} = \begin{bmatrix}
0.0575009 & -0.524268 & 0.28988 \\
-0.298951 & -0.771014 & -0.46527 \\
-0.47281 & -0.150827 & 0.793206 \\
0.826905 & -0.328529 & 0.265175
\end{bmatrix} \)

and therefore \( B' = \tilde{U} \sqrt{\tilde{\Sigma}} = \begin{bmatrix}
0.396999 & -2.36457 & 0.501221 \\
-2.06403 & -3.47744 & -0.804483 \\
-3.26439 & -0.680264 & 1.37151 \\
5.70914 & -1.48174 & 0.458505
\end{bmatrix} \)
We can then check \( B'B^T = \begin{bmatrix} 6 & 7 & 1 & 6 \\ 7 & 17 & 8 & -7 \\ 1 & 8 & 13 & -17 \\ 6 & -7 & -17 & 35 \end{bmatrix} \).

At this point, we will show that there is an orthogonal matrix \( Q \) such that \( B' = BQ \). The linear transformation that multiplies a vector by an orthogonal matrix is obtainable as a sequence of rotations and reflections \([8, \text{ p. 478}]\). So when we have shown that the coordinates found are for a molecule satisfying \( B' = BQ \), then the new molecule can be obtained from the original by rotation and reflection.

In order to find the necessary orthogonal matrix \( Q \), we must decompose \( B' \) and \( B'^T \) into their \( QR \) factorizations. A \( QR \) factorization on a matrix \( A \) expresses \( A \) as an orthogonal matrix \( Q \) and an upper triangular matrix \( R \). It is found by carrying out a Gram-Schmidt process on the column vectors of \( A \), \( \{a_1, a_2, \ldots, a_n\} \), to get our \( Q = \{u_1, u_2, \ldots, u_n\} \), and where \( \{u_1, u_2, \ldots, u_n\} \) are the columns of the orthonormal basis and we build \( R \), using values found during the Gram-Schmidt process,

\[
[r_{ij}] = \begin{cases} 
\langle a_j, u_i \rangle & \text{when } j \leq i \\
0 & \text{when } j > i 
\end{cases}
\]

The algorithm for this procedure is described below:

**Algorithm 1: Classical Gram-Schmidt Orthogonalization** [9]:

input: the columns of \( A = \{a_1, a_2, \ldots, a_n\} \)

output: an orthonormal basis \( \{u_1, u_2, \ldots, u_n\} \) for the span of these columns

for \( j = 1 \) to \( n \)

\[ u_j = a_j \]

for \( i = 1 \) to \( j - 1 \)

\[ r_{i,j} = \langle a_j, u_i \rangle \]

\[ u_j = u_j - r_{i,j} u_i \]

end

\[ r_{j,j} = \| u_j \| \]
\[ u_j = u_j/r_{j,j} \]

end.

Once we have the QR factorization for \( B^T \) and \( B^T \), then we can find the orthogonal matrix \( Q \) that acts as our linear transformation from \( B' \) to \( B \).

If we start with \( B^T = UR \) and \( (B')^T = U'R' \), then \( B = R^T U^T \) and \( B' = (R')^T (U')^T \).

When we do the QR factorization, we find that \( R^T = (R')^T \), thus we can say:

since \( B' = R^T (U')^T \)

\[ B' = BU(U')^T. \]

It follows that \( B' = BQ \), where \( Q = U(U')^T \).

**Example 12:** Using our familiar 5 atom configuration from Example 10:

\[
B = \begin{bmatrix}
1 & 2 & -1 \\
0 & 4 & 1 \\
-3 & 2 & 0 \\
5 & -1 & -3
\end{bmatrix}
\]

so \( B^T = \begin{bmatrix}
1 & 0 & -3 & 5 \\
2 & 4 & 2 & -1 \\
-1 & 1 & 0 & -3
\end{bmatrix} \), and

\[
B' = \begin{bmatrix}
0.396999 & -2.36457 & 0.501221 \\
-2.06403 & -3.47744 & -0.804483 \\
-3.26439 & -0.680264 & 1.37151 \\
5.70914 & -1.48174 & 0.458505
\end{bmatrix}
\]

so \( (B')^T = \begin{bmatrix}
0.396999 & -2.06403 & -3.26439 & 5.70914 \\
-2.36457 & -3.47744 & -0.680264 & -1.48174 \\
0.501221 & -0.804483 & 1.37151 & 0.458505
\end{bmatrix} \)

Gram-Schmidt process on \( B^T \) yields:
\[ U = \begin{bmatrix} 0.408248 & -0.392541 & -0.824163 \\ 0.816497 & 0.560772 & 0.137361 \\ -0.408248 & 0.729004 & -0.549442 \end{bmatrix} \]

and Gram-Schmidt process on \((B')^T\) yields:

\[ U' = \begin{bmatrix} 0.16205 & -0.850442 & -0.500488 \\ -0.96536 & -0.241739 & 0.0982005 \\ 0.204501 & -0.467238 & 0.860156 \end{bmatrix} \]

Calculating \(R\) and \(R'\) goes as follows:

\[
R = \begin{bmatrix}
\langle u_1, b_1 \rangle & \langle u_1, b_2 \rangle & \langle u_1, b_3 \rangle & \langle u_1, b_4 \rangle \\
0 & \langle u_2, b_2 \rangle & \langle u_2, b_3 \rangle & \langle u_2, b_4 \rangle \\
0 & 0 & \langle u_3, b_3 \rangle & \langle u_3, b_4 \rangle 
\end{bmatrix} = \\
\begin{bmatrix}
2.44949 & 2.85774 & 0.408248 & 2.44949 \\
0 & 2.97209 & 2.29917 & -4.71049 \\
0 & 0 & 2.74721 & -2.60985 
\end{bmatrix}
\]

E.g., \(\langle u_1, b_1 \rangle = 0.408248 \times 1 + 0.816497 \times 2 - 0.408248 \times 1 = 2.44949\)

From our definition of \(R\) as upper triangular, we know that \(\langle u_3, b_2 \rangle = 0\). We can check by calculating \(\langle u_3, b_2 \rangle = -0.824163 \times 0 + 0.137361 \times 4 - 0.549442 \times 1\) which does indeed equal zero.

\[
R' = \begin{bmatrix}
\langle u'_1, b'_1 \rangle & \langle u'_1, b'_2 \rangle & \langle u'_1, b'_3 \rangle & \langle u'_1, b'_4 \rangle \\
0 & \langle u'_2, b'_2 \rangle & \langle u'_2, b'_3 \rangle & \langle u'_2, b'_4 \rangle \\
0 & 0 & \langle u'_3, b'_3 \rangle & \langle u'_3, b'_4 \rangle 
\end{bmatrix} = \\
\begin{bmatrix}
2.44949 & 2.85774 & 0.408248 & 2.44949 \\
0 & 2.97209 & 2.29917 & -4.71049 \\
0 & 0 & 2.74721 & -2.60985 
\end{bmatrix}
\]
e.g.,

\[ \langle u'_2, b'_2 \rangle = -0.850442 \times -2.06403 + -0.241739 \times -3.47744 + -0.467238 \times -0.804483 = 2.971855 \]

(rounding error introduced)

Therefore, we see \( R = R' \) and so \( R^T = (R')^T \).

Calculating \( Q = U(U')^T \) we get

\[
Q = \begin{pmatrix}
0.812613 & -0.380122 & -0.441778 \\
-0.413273 & -0.910314 & 0.0230861 \\
-0.410932 & 0.163815 & -0.896827
\end{pmatrix}
\]

And we conclude by showing that \( B' = BQ \):

\[
B' = \begin{bmatrix}
1 & 2 & -1 \\
0 & 4 & 1 \\
-3 & 2 & 0 \\
5 & -1 & -3
\end{bmatrix}
\begin{pmatrix}
0.812613 & -0.380122 & -0.441778 \\
-0.413273 & -0.910314 & 0.0230861 \\
-0.410932 & 0.163815 & -0.896827
\end{pmatrix}
\]

\[
= \begin{pmatrix}
0.396999 & -2.36457 & 0.501221 \\
-2.06403 & 3.47744 & -0.804483 \\
-3.26439 & -0.680264 & 1.37151 \\
5.70914 & -1.48174 & 0.458505
\end{pmatrix}
\]

Example 13: Eleven atom molecule. Given the following:
$$A^o = \begin{bmatrix} 2 & 1 & -3 \\ 0 & -3 & 2 \\ 1 & 3 & -1 \\ -2 & 1 & -2 \\ 6 & -2 & -5 \end{bmatrix}, \quad T = \begin{bmatrix} -1 & 1 & 2 \\ -1 & 1 & 2 \\ -3 & 2 & 0 \\ 5 & -1 & -3 \\ 0 & 0 & 0 \end{bmatrix}, \quad A = A^o + T = \begin{bmatrix} 1 & 2 & -1 \\ -1 & -2 & 4 \\ 0 & 4 & 1 \\ -3 & 2 & 0 \\ 5 & -1 & -3 \\ 0 & 0 & 10 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 2 & -1 \\ -1 & -2 & 4 \\ 0 & 4 & 1 \\ -3 & 2 & 0 \\ 5 & -1 & -3 \\ 0 & 0 & 10 \end{bmatrix}.$$
Using Mathematica, the distance matrix $D = \begin{pmatrix}
0 & 3 \sqrt{5} & 3 & \sqrt{17} & \sqrt{29} & 3 \sqrt{14} & \sqrt{41} & \sqrt{26} & 3 \sqrt{2} & \sqrt{182} & \sqrt{6} \\
3 \sqrt{5} & 0 & \sqrt{46} & 6 & \sqrt{86} & \sqrt{41} & \sqrt{106} & 9 & 3 \sqrt{5} & 3 \sqrt{11} & \sqrt{21} \\
3 & \sqrt{46} & 0 & \sqrt{14} & \sqrt{66} & \sqrt{97} & 2 \sqrt{14} & 2 \sqrt{41} & \sqrt{21} & \sqrt{129} & \sqrt{17} \\
\sqrt{17} & 6 & \sqrt{14} & 0 & \sqrt{82} & \sqrt{113} & \sqrt{26} & 9 & \sqrt{53} & \sqrt{107} & \sqrt{13} \\
\sqrt{29} & \sqrt{86} & \sqrt{66} & \sqrt{82} & 0 & \sqrt{195} & \sqrt{94} & \sqrt{19} & \sqrt{35} & \sqrt{329} & \sqrt{35} \\
3 \sqrt{14} & \sqrt{41} & \sqrt{97} & \sqrt{113} & \sqrt{195} & 0 & 7 \sqrt{5} & 2 \sqrt{35} & 2 \sqrt{21} & \sqrt{74} & 10 \\
\sqrt{41} & \sqrt{106} & 2 \sqrt{14} & \sqrt{26} & \sqrt{94} & 7 \sqrt{5} & 0 & 5 \sqrt{5} & \sqrt{113} & \sqrt{213} & 3 \sqrt{5} \\
\sqrt{26} & 9 & \sqrt{41} & 9 & \sqrt{19} & 2 \sqrt{35} & 5 \sqrt{5} & 0 & 2 \sqrt{2} & \sqrt{278} & 2 \sqrt{10} \\
3 \sqrt{2} & 3 \sqrt{5} & \sqrt{21} & \sqrt{53} & \sqrt{35} & 2 \sqrt{21} & \sqrt{113} & 2 \sqrt{2} & 0 & \sqrt{194} & 2 \sqrt{6} \\
\sqrt{182} & 3 \sqrt{11} & \sqrt{129} & \sqrt{107} & \sqrt{329} & \sqrt{74} & \sqrt{213} & \sqrt{278} & \sqrt{194} & 0 & \sqrt{154} \\
\sqrt{6} & \sqrt{21} & \sqrt{17} & \sqrt{13} & \sqrt{35} & 10 & \sqrt{3} & 2 \sqrt{10} & 2 \sqrt{6} & \sqrt{154} & 0
\end{pmatrix}

We calculate $\hat{D}$ from the distance matrix and find $\hat{D} = \begin{pmatrix}
6 & -9 & 7 & 1 & 6 & -10 & 5 & 10 & 6 & -11 \\
-9 & 21 & -4 & -1 & -15 & 40 & -20 & -10 & 0 & 38 \\
7 & -4 & 17 & 8 & -7 & 10 & 3 & 8 & 10 & 21 \\
1 & -1 & 8 & 13 & -17 & 0 & 16 & -14 & -8 & 30 \\
6 & -15 & -7 & -17 & 35 & -30 & -7 & 28 & 12 & -70 \\
-10 & 40 & 10 & 0 & -30 & 100 & -50 & 0 & 20 & 90 \\
5 & -20 & 3 & 16 & -7 & -50 & 45 & -20 & -22 & -7 \\
10 & -10 & 8 & -14 & 28 & 0 & -20 & 40 & 28 & -42 \\
6 & 0 & 10 & -8 & 12 & 20 & -22 & 28 & 24 & -8 \\
-11 & 38 & 21 & 30 & -70 & 90 & -7 & -42 & -8 & 154
\end{pmatrix}.$

The nonzero eigenvalues of $\hat{D}$ are the diagonals for $\hat{\Sigma}$ and thus $\hat{\Sigma} = \begin{pmatrix}
277.995 & 0 & 0 \\
0 & 130.386 & 0 \\
0 & 0 & 46.6191
\end{pmatrix},$

so $\sqrt{\hat{\Sigma}} = \begin{pmatrix}
16.6732 & 0 & 0 \\
0 & 11.4187 & 0 \\
0 & 0 & 6.82782
\end{pmatrix}.$
Calculating $\tilde{U}$ we get:

$$
\begin{pmatrix}
-0.0686558 & -0.0138646 & -0.316318 \\
0.221725 & -0.123593 & 0.338494 \\
0.0774119 & -0.0166354 & -0.572843 \\
0.105676 & 0.237419 & -0.233691 \\
-0.313802 & -0.241217 & 0.0288387 \\
0.510231 & 0.458193 & 0.0739199 \\
-0.118613 & 0.540792 & -0.251842 \\
-0.171768 & -0.431063 & -0.40297 \\
-0.00806786 & -0.37415 & -0.350568 \\
0.725616 & 0.203721 & -0.218178
\end{pmatrix}
$$

Finally, we calculate $B' = \tilde{U} \sqrt{\Sigma}$ and get:

$$
\begin{pmatrix}
-1.14471 & -0.158315 & -2.15976 \\
3.69686 & -1.41127 & 2.31118 \\
1.2907 & -0.189955 & -3.91127 \\
1.76195 & 2.71101 & -1.5956 \\
-5.23208 & -2.75438 & 0.196906 \\
8.50717 & -5.23195 & 0.504712 \\
-1.97765 & 6.17512 & -1.71953 \\
-2.66392 & -4.92217 & -2.75141 \\
-0.134517 & -4.27229 & -2.39362 \\
12.0983 & 2.32622 & -1.48968
\end{pmatrix}
$$

A scatter plot for $B' = \text{...}$
1. Schnell, S., *Centre for Mathematical Biology*,
   http://www.maths.ox.ac.uk/cmb/Research/index.html accessed 5/21/06.

   http://www.netsci.org/Science/Compchem/feature17b.html accessed 5/31/06.


