LECTURE 26

I. Summary of
   Inner Product vs Metric vs Duality

II. Gram-Schmidt Orthonormalization

III. Relation Between Oblique and
      Orthogonal Basis
1) Inner Product vs. Metric vs Duality. 26.1

Every finite dimensional vector space has a set of coordinate functions \( \{ e_i \} \) whose isomorphs are dual to the coordinate lines of a chosen basis \( \{ e_i \} \):

\[
< \omega \delta | e_i > = \delta_i^\omega
\]

A vector space with a metric \( (g(...)...) \) [see Lecture 9] or an inner product \( (\ldots,\ldots) \) [see the previous Lecture 25] structure implies a scalar value for every pair of vectors. It thereby puts into numerical form observed mutual properties such as the angle and/or orthogonality between them, the squared lengths of each, and others.
An inner product is a special case of a metric. Indeed, one has

\[(u, v) = g(u, v)\]

\[(v, u) = (u, v) = g(v, v) = g(u, u)\]

although by an inner product one always understands it to have the positive definite property

\[(u, u) > 0 \text{ whenever } u \neq 0.\]

By contrast for some metrics (e.g., the Minkowski spacetime metric) a vector space has elements which are characterized by all three possibilities

\[g(u, u) > 0 \text{; } g(u, v) = 0 \text{; } g(u, u) < 0.\]

However, unlike for an inner product,
often for a metric, it is usually understood that it is defined on a real vector space.

Both a metric and an inner product assign a unique element

\[ u \in V \mapsto (u, \ldots) = g(u, \ldots) = \langle u \mid \ldots \rangle \in V^* \]

to each vector \( u \). With the introduction of the Dirac notation one has therefore

\[ (u, v) = g(u, v) = \langle u \mid v \rangle \quad \forall u, v \in V \]

The Dirac bracket notation holds whether or not a metric (or an inner product) is defined on \( V \), i.e., whether or not there is a metric (or inner product) induced isomorphism \( \bar{u} \in V \mapsto \langle u \mid \bar{u} \rangle \in V^* \) between \( V \) and \( V^* \).
Most, if not all text books on quantum mechanics (including the one by Dirac himself) assume such a correspondence. However, such an assumption is only valid if one can arrive at it on the basis of observational evidence.
II. The Gram-Schmidt Orthonormalization Process.

A) Computational Simplicity.

The advantage of an orthogonal basis

\[ \{ \mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n \} \quad \mathbf{v}_i \cdot \mathbf{v}_j = 0 \quad i \neq j \]

at compared to an oblique basis

\[ \{ \mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_n \} \quad \mathbf{u}_i \cdot \mathbf{u}_j = q_{ij} \]

lies in the simplicity of the orthogonal basis representation for any vector \( \mathbf{x} \)

\[
\mathbf{x} = \mathbf{v}_1 \left( \frac{\mathbf{v}_1 \cdot \mathbf{x}}{\| \mathbf{v}_1 \|^2} \right) \mathbf{v}_1 + \mathbf{v}_2 \left( \frac{\mathbf{v}_2 \cdot \mathbf{x}}{\| \mathbf{v}_2 \|^2} \right) \mathbf{v}_2 + \cdots + \mathbf{v}_n \left( \frac{\mathbf{v}_n \cdot \mathbf{x}}{\| \mathbf{v}_n \|^2} \right) \mathbf{v}_n
\]

or equivalently

\[
\mathbf{x} = \mathbf{v}_1 \frac{\mathbf{v}_1 \cdot \mathbf{x}}{\mathbf{v}_1 \cdot \mathbf{v}_1} + \mathbf{v}_2 \frac{\mathbf{v}_2 \cdot \mathbf{x}}{\mathbf{v}_2 \cdot \mathbf{v}_2} + \cdots + \mathbf{v}_n \frac{\mathbf{v}_n \cdot \mathbf{x}}{\mathbf{v}_n \cdot \mathbf{v}_n}
\]

as compared to the computational complexity for

\[
\mathbf{x} = \mathbf{v}_1 \sum_{j=1}^{n} g_{ij}^2 (\mathbf{u}_j \cdot \mathbf{x}) + \mathbf{v}_2 \sum_{j=1}^{n} g_{ij}^2 (\mathbf{u}_j \cdot \mathbf{x}) + \cdots
\]

or

\[
\mathbf{x} = \mathbf{v}_1 \frac{ \mathbf{v}_1 \cdot \mathbf{x} }{ \mathbf{v}_1 \cdot \mathbf{v}_1 } + \mathbf{v}_2 \frac{ \mathbf{v}_2 \cdot \mathbf{x} }{ \mathbf{v}_2 \cdot \mathbf{v}_2 } + \cdots + \mathbf{v}_n \frac{ \mathbf{v}_n \cdot \mathbf{x} }{ \mathbf{v}_n \cdot \mathbf{v}_n }
\]
where
\[
[ q^{-2} ] = \left[ [u_i, u_k] \right]^{-1} \]
\[
\text{Notation } \rightarrow \langle u_i | u_k \rangle \quad q^{-\frac{1}{2}}
\]
is the inverse of the matrix of the inner products of the \( \tilde{u}_i \)'s.


However, given an arbitrary in general oblique basis, an orthogonal, in fact, an orthonormal basis can be constructed by a sequential process as expressed by the following:

**Theorem 26.1 (Gram-Schmidt Orthogonalization)**

(P343 in J.R.A.)

Let \( \{ u_1, u_2, \ldots \} \) be a linearly independent set of vectors in an inner product space.
Then the vectors

\[ \mathbf{v}_1 = \mathbf{u}_1 \]

\[ \mathbf{v}_k = \mathbf{u}_k - \sum_{i=1}^{k-1} \mathbf{v}_i \frac{\langle \mathbf{v}_i, \mathbf{u}_k \rangle}{\| \mathbf{v}_i \|^2}, \quad 2 \leq k \leq n \]

are mutually orthogonal

\[ \langle \mathbf{v}_k, \mathbf{v}_\ell \rangle = 0, \quad k \neq \ell, \]

and they form an orthogonal basis whenever \( k = n \).

Proof via construction by removing all orthogonal projections of an obliquely directed:

**Step 1:** Let \( \mathbf{v}_1 = \mathbf{u}_1 \)

so that

\[ e_1 = \frac{\mathbf{v}_1}{\| \mathbf{v}_1 \|} \]

is the corresponding unit vector.
Step 2: Obtain $v_2$ by removing the orthogonal projection from $u_2$:

$$v_2 = u_2 - e_1 \langle e_1 | u_2 \rangle$$

$$= u_2 - \frac{v_1 \langle v_1 | u_2 \rangle}{||v_1||^2}$$

$e_1 \langle e_1 | u_2 \rangle$ = projection onto $v_1$-direction

The normalized unit vector $u_2$

$$e_2 = \frac{v_2}{||v_2||}$$

Two comments:

(i) $v_2 \neq 0$! Why? Because $\{u_2, v_1\}$ is a linearly independent set.

(ii) $\langle v_1 | v_2 \rangle = 0$
Step 3
obtain $v_3$ by removing the two orthogonal projections from $u_3$

$$v_3 = u_3 - e_1 <e_1 | u_3> - e_2 <e_2 | u_3>$$

$$= u_3 - \frac{v_1}{||v_1||^2} <v_1 | u_3> - \frac{v_2}{||v_2||^2} <v_2 | u_3>$$

so that

$$e_3 = \frac{v_3}{||v_3||}$$

is a unit vector

Two comments

(i) $v_3 \neq 0$; Why? Because $\{u_3, v_1, v_2\}$ is a lin. indep. set

(ii) $<v_1 | v_3> = 0$

$<v_2 | v_3> = 0$
Step k

obtain \( v_k \) by removing the \( k-1 \) orthogonal projections from \( u_k \),

\[
    v_k = u_k - e_1 \langle e_1 | u_k \rangle - \cdots - e_{k-1} \langle e_{k-1} | u_k \rangle \\
   = u_k - \frac{v_1 \langle v_1 | u_k \rangle}{\| v_1 \|^2} - \cdots - \frac{v_{k-1} \langle v_{k-1} | u_k \rangle}{\| v_{k-1} \|^2}
\]

\[
    u_k^\perp = \sum_{i=1}^{k-1} \frac{v_i \langle v_i | u_k \rangle}{\| v_i \|^2}
\]

Three comments

(i) \( u_k^\perp \neq 0 \)

(ii) \( \langle v_i | u_k \rangle = 0 \) for \( i \neq k \)

(iii) \( \langle e_i | e_j \rangle = \delta_{ij} \) for \( i, j = 1, 2, \ldots, k \).

i.e., \( \{ e_i = \frac{v_i}{\| v_i \|} \}_{i=1}^{k} \) forms an o.n. set.
III Relation Between Oblique and Orthogonal Basis

The G-S process replaces the old oblique basis \( \{u_1, u_2, \ldots, u_n\} \) with the new orthonormal basis \( \{e_1, e_2, \ldots, e_n\} \).

This replacement is expressed by means of a linear transformation

\[
u_1 = e_1, \frac{v_1}{||v_1||} \]

\[
u_2 = e_2, \frac{v_1^\top u_2}{||v_1||} + e_2, \frac{v_2}{||v_2||} \]

\[
u_k = e_k, \frac{v_1^\top u_k}{||v_1||} + e_2, \frac{v_2^\top u_k}{||v_2||} + \ldots + e_k, \frac{v_k}{||v_k||} \]

Rewriting this vectorial relative to standard basis. The matrix whose columns make up the linearly indep. set \( \{u_1, \ldots, u_n\} \) is
\[
\begin{bmatrix}
u_1 & v_2 & \cdots & v_k \\
\end{bmatrix} =
\begin{bmatrix}
e_1 & e_2 & \cdots & e_k \\
\end{bmatrix}
\begin{bmatrix}
\|v_1\| & \langle v_1, v_2 \rangle & \langle v_1, v_3 \rangle & \cdots & \langle v_1, v_k \rangle \\
0 & \|v_2\| & \langle v_2, v_3 \rangle & \cdots & \langle v_2, v_k \rangle \\
0 & 0 & \ddots & \ddots & \ddots \\
0 & 0 & 0 & \ddots & \|v_k\| \\
\end{bmatrix}
\]

Matrix of maximal rank \(k\) = Matrix with orthonormal columns [upper triangular matrix]

\[U = OR\]

\[(n \times k) = (n \times k) \cdot (k \times k)\]

\[U_{ij} = \sum_{i=1}^{k} e_i \times R_{ij}\]

Thus we have the following theorem:

**Theorem**

Let \(U\) be an \(n \times k\) matrix with a lin. indep. set of columns. Then \(U\) can be factored as \(U = QR\), where \(Q\) is an \(n \times k\) matrix with o.n. columns and \(R\) is an invertible \(k \times k\) upper triangular matrix.