LECTURE 26

I. Summary of
Inner Product vs Metric vs Duality

II. Gram-Schmidt Orthonormalization

III Relation Between Oblique and
Orthogonal Basis; QR Decomposition

I.) Inner Product vs. Metric vs Duality. 26.1

Every finite dimensional vector space has a set of coordinate functions $\{\underset{\sim}{\omega}^j\}$ whose isograms are dual to the coordinate lines of a chosen basis $\{e_i\}$:

$$\langle \underset{\sim}{\omega}^j | e_i \rangle = \delta^j_i$$

A vector space with a metric ($g(\ldots,\ldots)$) [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 orthogonality between them, the squared lengths of each, and others.

26.2

An inner product is a special case of a metric. Indeed, one has

$$(u,v) = g(u,v)$$

$$(v,u) = \overline{(u,v)} = g(v,u) = \overline{g(u,v)}$$

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

$$(u,u) > 0 \text{ whenever } u \neq \vec{0}.$$

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

$$g(u,u) > 0; \; g(u,u) = 0, \; g(u,u) < 0.$$

However, unlike for an inner product,

for a metric, it is ~~usually~~ often understood that it is defined on a real vectorspace.

Both a metric and an inner product assign the same unique element

$$(u, \ldots) = g(u, \ldots) \equiv \langle u | \quad \in V^*$$

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

$$(u,v) = g(u,v) \equiv \langle u | v \rangle \quad \forall\, u, v \in V$$

The Dirac bracket notion 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

$$\vec{u}\ (\in V) \rightsquigarrow \langle u |\ (\in V^*)$$

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

$$\{v_1, v_2, \ldots, v_n : v_i \cdot v_j = 0, i \neq j\}$$

at compared to an oblique basis

$$\{u_1, u_2, \ldots, u_n ; u_i \cdot u_j = g_{ij}\}$$

lies in the simplicity of the orthogonal basis representation for any vector x

$$\boxed{\begin{aligned} x &= v_1 \frac{(v_1, x)}{\|v_1\|^2} + v_2 \frac{(v_2, x)}{\|v_2\|^2} + \cdots + v_n \frac{(v_n, x)}{\|v_n\|^2} \\ &\text{or equivalently} \\ x &= v_1 \frac{v_1 \cdot x}{v_1 \cdot v_1} + v_2 \frac{v_2 \cdot x}{v_2 \cdot v_2} + \cdots + v_n \frac{v_n \cdot x}{\|v_n\|^2} \end{aligned}}$$

as compared to the computational complexity for

$$x = u_1 \sum_{j=1}^{n} g^{1j}(u_1, x) + u_2 \sum_{j=1}^{n} g^{2j}(u_2, x) + \cdots$$

$$= u_1 \sum_{j=1}^{n} g^{1j}\; u_1 \cdot x + u_2 \sum_{j=1}^{n} g^{2j}\; u_2 \cdot x + \cdots$$

where

$$[g^{ij}] = [\underbrace{(u_j, u_k)}_{\substack{\text{|||} \\ \langle u_j | u_k \rangle}}]^{-1} = [\underbrace{u_j \cdot u_k}_{\substack{\text{|||} \\ g_{jk}}}]^{-1}$$

Notation $\rightarrow$

is the inverse of the matrix of the inner products of the w_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)

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

Then the vectors

$v_1 = u_1$

$$v_k = u_k - \sum_{i=1}^{k-1} v_k \frac{\langle v_k | u_i \rangle}{\|v_k\|^2} \qquad 2 \le k \le n$$

are mutually orthogonal

$\langle v_k | v_\ell \rangle = 0 \quad k \neq \ell,$

and

$\{v_1, v_2, \ldots, v_n\}$

is an orthogonal basis whenever $k=n$

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proof via construction by removing all orthogonal projections of an obliquely directed.

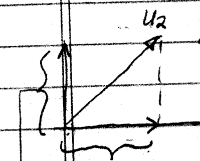
Step 1: Let $v_1 = u_1$
so that

$$e_1 = \frac{v_1}{\|v_1\|}$$

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

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

The normalized unit vector is

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

Two comments:

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

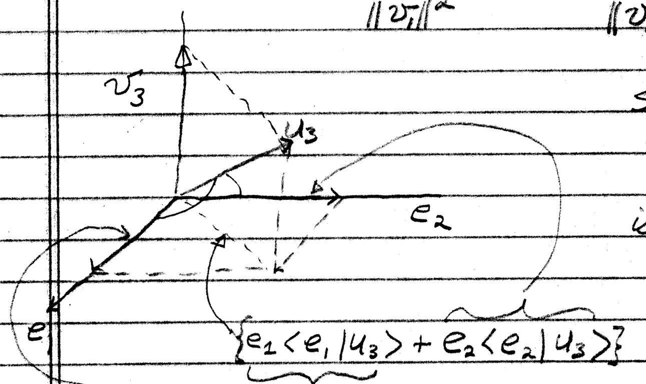
(ii) $\langle v_1 | v_2 \rangle = 0$

Step 3

Obtain v_3 by removing the two orthogonal projections from u_3,

$$v_3 = u_3 - e_1\langle e_1|u_3\rangle - e_2\langle e_2|u_3\rangle$$

$$= u_3 - \frac{v_1\langle v_1|u_3\rangle}{\|v_1\|^2} - \frac{v_2\langle v_2|u_3\rangle}{\|v_2\|^2}$$



so that $e_3 = \dfrac{v_3}{\|v_3\|}$ 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) $\langle v_1|v_3\rangle = 0$

$\langle v_2|v_3\rangle = 0$

Step k

Obtain v_k by removing the $k-1$ orthogonal projections from u_k,

$$v_k = u_k - e_1\langle e_1|u_k\rangle - \cdots - e_{k-1}\langle e_{k-1}|u_k\rangle$$

$$= u_k - \frac{v_1\langle v_1|u_k\rangle}{\|v_1\|^2} - \cdots \frac{v_{k-1}\langle v_{k-1}|u_k\rangle}{\|v_{k-1}\|^2}$$

$$\boxed{v_k = u_k - \sum_{i=1}^{k-1} \frac{v_i\langle v_i|u_k\rangle}{\|v_i\|}}$$

Three comments

(i) $v_k \neq \vec{0}$

(ii) $\langle v_\ell|v_k\rangle = 0$ for $\ell \neq k$

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

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 $\{e_1, e_2, \ldots\} = \left\{\frac{v_1}{\|v_1\|}, \frac{v_2}{\|v_2\|}, \ldots\right\}$

This replacement is expressed by means of a linear transformation

$$u_1 = \overbrace{e_1\|v_1\|}^{v_1}$$

$$u_2 = e_1\frac{\langle v_1|u_2\rangle}{\|v_1\|} + \overbrace{e_2\|v_2\|}^{v_2}$$

$$\vdots$$

$$u_k = e_1\frac{\langle v_1|u_k\rangle}{\|v_1\|} + e_2\frac{\langle v_2|u_k\rangle}{\|v_2\|} + \cdots \overbrace{e_k\|v_k\|}^{v_k}$$

Rewriting this vectorial relative to standard basis. The matrix whose columns make up the linearly indep. set $\{u_1, \ldots, u_k\}$ is

$$\begin{bmatrix} \vdots & \vdots & & \vdots \\ u_1 & u_2 & \cdots & u_k \\ \vdots & \vdots & & \vdots \end{bmatrix} = \begin{bmatrix} \vdots & \vdots & & \vdots \\ e_1 & e_2 & \cdots & e_k \\ \vdots & \vdots & & \vdots \end{bmatrix} \begin{bmatrix} \|v_1\| & \langle v_1|u_2\rangle/\|v_1\| & \cdots & \langle v_1|u_k\rangle/\|v_1\| \\ 0 & \|v_2\| & \cdots & \langle v_2|u_k\rangle/\|v_2\| \\ \vdots & \vdots & & \vdots \\ 0 & 0 & & \|v_k\| \end{bmatrix}$$

$$\begin{bmatrix} \text{matrix of} \\ \text{maximal} \\ \text{rank } k \end{bmatrix} = \begin{bmatrix} \text{matrix with} \\ \text{orthonormal} \\ \text{columns} \end{bmatrix} \begin{bmatrix} \text{upper} \\ \text{triangular} \\ \text{matrix} \end{bmatrix}$$

(i.e. set of lin indep columns)

$$U \quad = \quad Q \quad R$$

$$(n\times k) = (n\times k) \cdot (k\times k)$$

$$u_j = \sum_{i=1}^{k} e_i \times R_{ij} \qquad j = 1, \ldots, k$$

Thus we have the following

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.