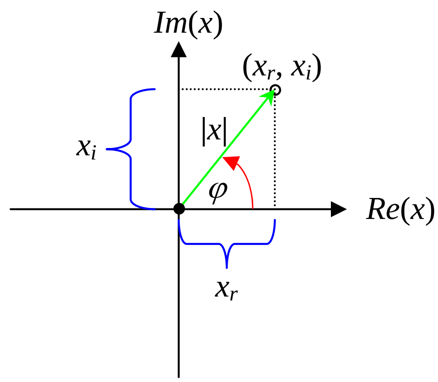
Supplemental Handout #1

Orthogonal Functions & Expansions

Consider a function $f(x)$ which is defined on the interval $a \le x \le b$. The function $f(x)$ and its independent variable, x *may* be real, but it could also be *complex*, i.e. $\boxed{x \equiv x_r + i x_i}$, where $i \equiv \sqrt{-1}$ and $\boxed{x^* \equiv x_r - i x_i}$ = the complex conjugate of x.

$$i^* \equiv -i = -\sqrt{-1}$$
$$i^* i = i i^* = +1$$

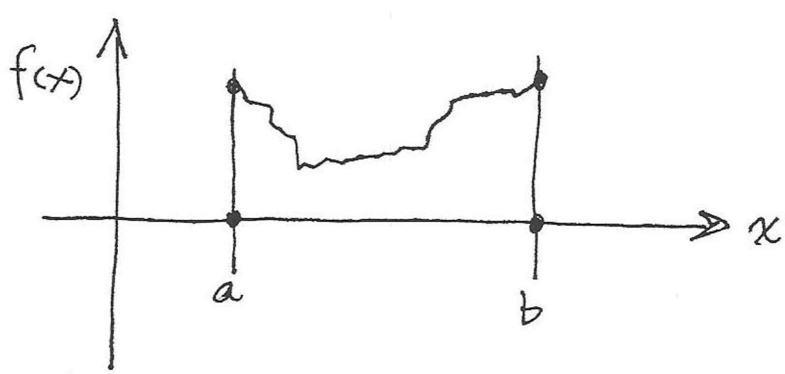
$$x = |x| e^{i\varphi} = |x|(\cos\varphi + i\sin\varphi)$$
$$x_r = |x|\cos\varphi \qquad x_i = |x|\sin\varphi$$



$$|x| \equiv \sqrt{x^* x} = \sqrt{x_r^2 + x_i^2}$$

$$\varphi = \tan^{-1}\left(\frac{x_i}{x_r}\right)$$

The function $f(x)$ *must* be mathematically "well-behaved" on the interval $a \le x \le b$ - i.e. it must be single- (not multiple-) valued, and (at least) be piece-wise continuous as well as be finite-valued everywhere – i.e. not singular (infinite) on the interval $a \le x \le b$:
e.g.



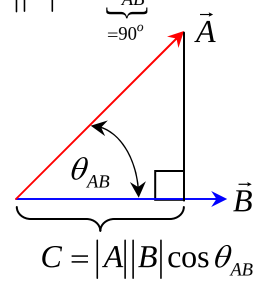
Mathematically we can express $f(x)$ as a specific linear combination of *orthonormal* functions, $u_n(x)$:

$$f(x) = a_0 u_0(x) + a_1 u_1(x) + a_2 u_2(x) + a_3 u_3(x) + \ldots$$
$$= \sum_{n=0}^{\infty} a_n u_n(x)$$

The a_n coefficients are pure numbers – either real or complex – one is associated with each of the orthonormal functions $u_n(x)$.

The orthonormal functions, $u_n(x)$ are very special functions – in general, they are polynomial functions of *x*, but they have very special properties:

1) The $u_n(x)$ are *orthonormal* to each other – i.e. mutually perpendicular to each other, analogous to a vector dot product (also known as an *inner product*): $C = \vec{A}\bullet\vec{B} = |\vec{A}||\vec{B}|\cos\underbrace{\theta_{AB}}_{=90^o} = 0$



Here, the inner product of the $u_n(x)$ functions is defined over the interval $a \le x \le b$ as: $\boxed{\langle u_m | u_n \rangle \equiv \int_a^b u_m^*(x)\cdot u_n(x)\,dx}$

2) The $u_n(x)$ are *normalized* functions on the interval $a \le x \le b$,
i.e. $\langle u_n | u_n \rangle = \int_a^b u_n^*(x)\cdot u_n(x)\,dx = \int_a^b |u_n(x)|^2\,dx = 1$ (for *all* *n*: $n = 0,1,2,3,\ldots$)

$|u_n(x)|^2 = u_n^*(x)\cdot u_n(x)$

Because the $u_n(x)$ are *orthonormal* functions, this means that on the interval $a \le x \le b$:

$$\langle u_m | u_n \rangle = \int_a^b u_m^*(x)\cdot u_n(x)\,dx = \begin{pmatrix} 0 \text{ if } m \ne n \\ 1 \text{ if } m = n \end{pmatrix}$$

$u_n(x)$ *orthogonality* on interval $a \le x \le b$:	$\int_a^b u_m^*(x)\cdot u_n(x)\,dx = 0 \Leftarrow u_m(x) \perp \text{ to } u_n(x)$
$u_n(x)$ *normalized* on interval $a \le x \le b$:	$\int_a^b u_n^*(x)\cdot u_n(x)\,dx = \int_a^b |u_n(x)|^2\,dx = 1$

We define a mathematical function known as the Kroenecker δ-function, represented by the symbol, δ_{nm} which has the following properties:

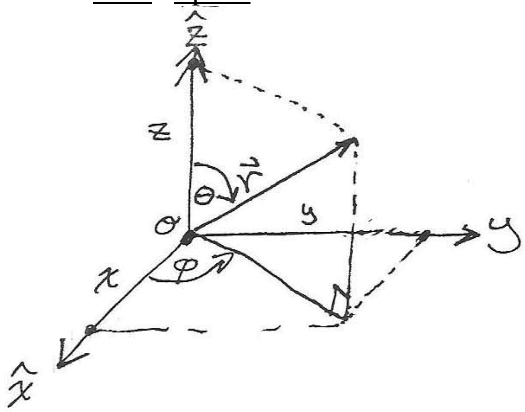
Kroenecker δ-function	$\delta_{nm} \equiv 0$, if $n \ne m$ $\delta_{nm} \equiv 1$, if $n = m$

Then:

$$\boxed{\langle u_m | u_n \rangle \equiv \int_a^b u_m^*(x)\cdot u_n(x)\,dx = \delta_{nm} \quad \text{on the interval } a \le x \le b}$$

The orthonormal functions, $u_n(x)$ are said to form an *orthonormal basis* – i.e. the $u_n(x)$ behave like mutually-orthogonal (mutually-perpendicular) unit-vectors (analogous to the $\hat{x}, \hat{y}, \hat{z}$ unit vectors in 3-*D* "real" space), however, this mathematical space is infinite-dimensional, known as Hilbert Space.

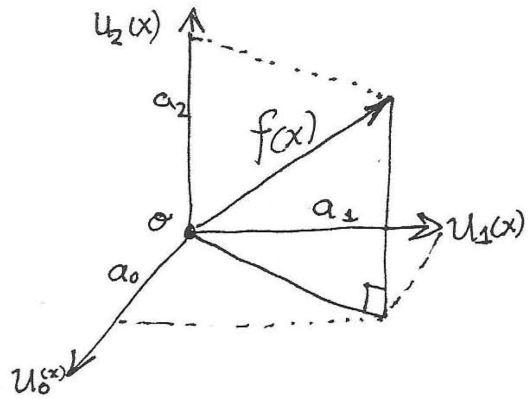
3 – *D*
“Real” Space:



$$\vec{r} = x\hat{x} + y\hat{y} + z\hat{z}$$

$$|\vec{r}| = \sqrt{x^2 + y^2 + z^2}$$

Hilbert Space:
(∞-dimensional)



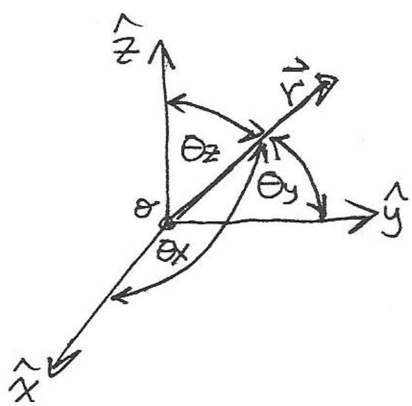
$$f(x) = a_0 u_0(x) + a_1 u_1(x) + a_2 u_2(x) + ... = \sum_{n=0}^{\infty} a_n u_n(x)$$

Just as in 3-*D* “real” space, the coefficients *x*,*y*,*z* are the projections of the vector, $\vec{r}$ onto the $\hat{x}, \hat{y}, \hat{z}$ orthonormal axes/basis vectors, respectively, i.e.

$$x = \vec{r} \cdot \hat{x} = |\vec{r}| \cos\theta_x \qquad (|\hat{x}| = 1) \qquad (\cos\theta_x = \hat{r} \cdot \hat{x} = x\text{-direction cosine})$$

$$y = \vec{r} \cdot \hat{y} = |\vec{r}| \cos\theta_y \qquad (|\hat{y}| = 1) \qquad (\cos\theta_y = \hat{r} \cdot \hat{y} = y\text{-direction cosine})$$

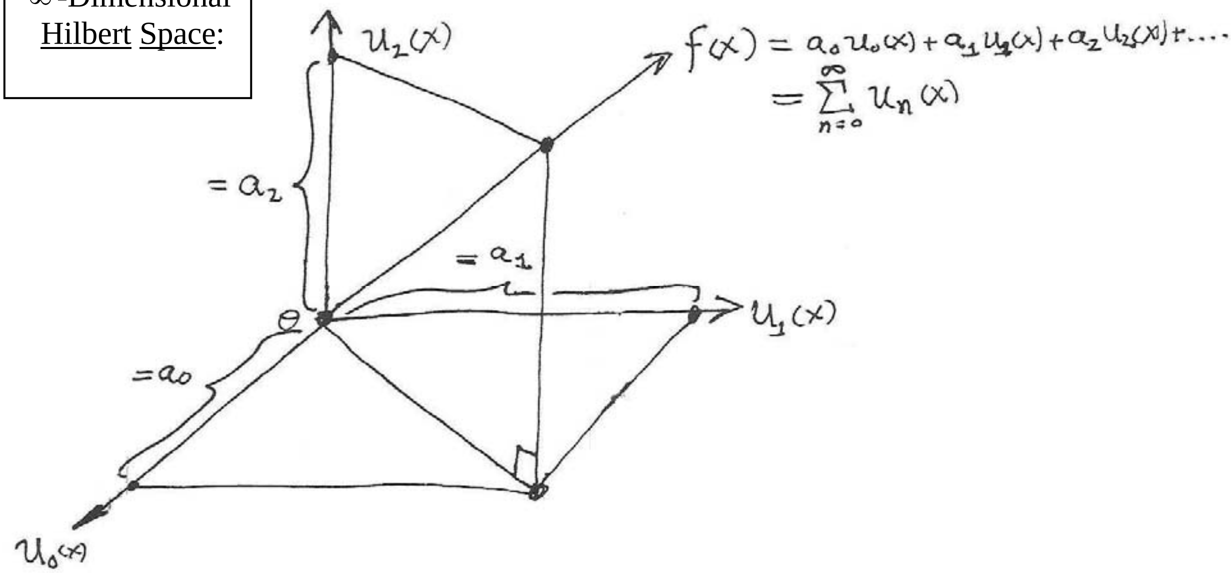
$$z = \vec{r} \cdot \hat{z} = |\vec{r}| \cos\theta_z \qquad (|\hat{z}| = 1) \qquad (\cos\theta_z = \hat{r} \cdot \hat{z} = z\text{-direction cosine})$$



Direction Cosines in 3-D “Real” Space

In Hilbert Space (∞-dimensional) the coefficients $a_n\left(a_0, a_1, a_2, a_3 ...\right)$ (may be real or complex, if $u_n(x)$ are real or complex) are the projections of $f(x)$ = “vector” in Hilbert Space, onto the $u_n(x)$ orthonormal axis/basis vectors, respectively, i.e.

∞-Dimensional <u>Hilbert</u> <u>Space</u>:



n.b. The orthonormal functions, $u_n(x)$ are said to be <u>complete</u> - completely "spanning" the ∞-dimensional Hilbert space.

$\Rightarrow$ This means that *<u>any</u>* arbitrary, but well-behaved (see above) function, $f(x)$ can be exactly/ perfectly represented by an appropriate linear combination of the $u_n(x)$, i.e. $f(x) = \sum_{n=0}^{\infty} a_n u_n(x)$

In order to determine the coefficients a_n (on the interval $a \le x \le b$), we take <u>inner products</u>/dot-products of $u_n(x)$ with $f(x)$:

Project out n^{th} coefficient, a_n from $f(x)$

$$a_n = \langle u_n(x) | f(x) \rangle = \int_a^b u_n^*(x) \cdot f(x)\, dx$$

$$a_n = \int_a^b u_n^*(x) \cdot \left\{ \sum_{k=0}^{\infty} a_k u_k(x) \right\}$$

$$= \int_a^b u_n^*(x) \cdot \left[\underset{=0}{a_0 u_0(x)} + \underset{=0}{a_1 u_1(x)} + \ldots a_n u_n(x) \ldots \right] dx$$

$$a_k \int_a^b u_n^*(x) u_k(x) = 0 \text{ if } k \ne n$$

$$= a_0 \overbrace{\int_a^b u_n^*(x) u_0(x)\, dx}^{=0} + a_1 \overbrace{\int_a^b u_n^*(x) u_1(x)\, dx}^{=0} + \ldots + a_n \int_a^b u_n^*(x) u_n(x)\, dx$$

$$= a_n \underbrace{\int_a^b u_n^*(x) u_n(x)\, dx}_{=1} = a_k \delta_{nk} \qquad \begin{pmatrix} \delta_{nk} = 0 \text{ if } n \ne k \\ \delta_{nk} = 1 \text{ if } n = k \end{pmatrix}$$

Let's consider a real function $f(x)$ on the real interval $a \le x \le b$. We know that it is possible to exactly represent $f(x)$, (well-behaved) on the interval $a \le x \le b$ by a power series expansion:

$$f(x) = a_0 x^0 + a_1 x^1 + a_2 x_2^2 + a_3 x^3 + \ldots = \sum_{n=0}^{\infty} a_n x^n$$

because the x^n polynomials form a *complete set* on the real, ∞-dimensional space $\mathbb{R}^n$.

However, the polynomial functions x^n do *not* form an orthogonal basis – i.e. the x^n are *not* mutually perpendicular to each other in the ∞-dimensional Hilbert Space $\mathbb{R}^n$.

On the other hand, certain *appropriate* linear combinations of the x^n *do* form an orthonormal basis for the real, ∞-dimensional space $\mathbb{R}^n$.

For example, the Fourier functions (sines & cosines) $\left\{ \begin{matrix} \sin(nx),\ \cos(nx) \\ n = 0,1,2,3\ldots \end{matrix} \right\}$ form an orthonormal basis for $\mathbb{R}^n$ on the unit interval $-1 \le x \le 1$:

$$\sin(x) = \frac{x}{1!} - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \ldots = \sum_{k=odd\#}^{\infty} \left(-1^{\frac{(k-1)}{2}} \frac{x^k}{k!} \right) = \sum_{\ell=1}^{\infty} (-1)^{\ell-1} \frac{x^{2\ell}}{(2\ell-1)!} \qquad k = 2\ell - 1$$

$$\cos(x) = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \ldots = \sum_{k=even\#}^{\infty} (-1)^{\left(\frac{k}{2}\right)} \frac{x^k}{k!} = \sum_{\ell=0}^{\infty} (-1)^{\ell} \frac{x^{2\ell}}{(2\ell)!} \qquad k = 2\ell$$

where: $k! \equiv k(k-1)(k-2)\ldots 3\cdot 2\cdot 1$ and $0! = 1$, $1! = 1$, $2! = 2$, $3! = 6$, etc…

Many other polynomial functions of x form an orthonormal basis for $\mathbb{R}^n$:

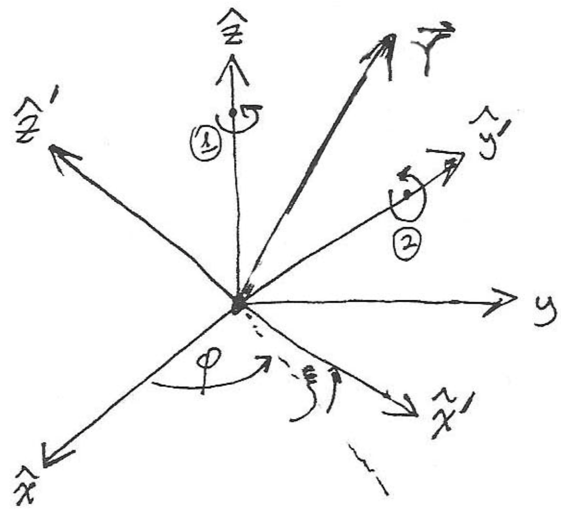
We simply/just list these for now:		If origin $x = 0$ is excluded must include:	
Legendre Functions/Polynomials:	$P_n(x)$	$Q_n(x)$	(singular @ $x = 0$)
Tschebychev Polynomials:	$T_n(x)$	$U_n(x)$	"
Jacobi/Elliptic Polynomials:	$K_n(x)$	$K'_n(x)$	"
Bessel Functions (1st & 2nd kind):	$J_n(x)$	$N_n(x)$	"
Hermite Polynomials:	$H_n(x)$	$H'_n(x)$	"
Laguerre Polynomials:	$L_n(x)$	$L'_n(x)$	"

etc…

The procedure for constructing a complete set of *orthonormal* basis vectors, e.g. in $\mathbb{R}^n$ is known the Gram-Schmidt ortho-normalization procedure.

The Fourier Functions/Legendre/Tschebychev/Jacobi/Bessel/Hermite Polynomials are all related to each other – by orthogonal transformations – i.e. rotations of basis vectors in ∞ – dimensional Hilbert Space – to another set of orthonormal basis vectors (e.g. Legendre Polynomials).

Rotations in Real 3-*D* Space: $= \overbrace{x\hat{x} + y\hat{y} + z\hat{z}}^{\vec{r} \text{ expressed in } x-y-z \text{ basis}} = \overbrace{x'\hat{x}' + y'\hat{y} + z'\hat{z}'}^{\vec{r} \text{ expressed in } x'-y'-z' \text{ basis}}$



$x'-y'-z'$ basis is related to $x-y-z$ basis by sequence of rotations (e.g. φ about $\hat{z}$ axis, then by ξ about new $\hat{y}$ axis:

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} Rotation \\ Matrix \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$X' = RX$$

Similarly, orthonormal bases in $\mathbb{R}^n$ are related to each other by orthogonal transformations in $\mathbb{R}^n$ space $X' = \mathbb{R}X$:

$$f(x) = \sum_{n=0}^{\infty} a_n u_n(x) = \sum_{n=0}^{\infty} b_n u_n'(x)$$