Supplemental Handout #1

Orthogonal Functions & Expansions

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

\[
\begin{align*}
  i^* & = -i = -\sqrt{-1} \\
  i^*i & = i(-i) = -1 = +1
\end{align*}
\]

\[
x = |x|e^{i\phi} = |x|(\cos \phi + i \sin \phi)
\]

\[
x_r = |x|\cos \phi \quad x_i = |x|\sin \phi
\]

The function \( f(x) \) must be mathematically “well-behaved” on the interval \( a \leq x \leq b \) - 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 \( a \leq x \leq b \):

For example,

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

\[
f(x) = a_0u_0(x) + a_1u_1(x) + a_2u_2(x) + a_3u_3(x) + \ldots
\]

\[
= \sum_{n=0}^{\infty} a_nu_n(x)
\]

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**): 
\[
C = \vec{A} \cdot \vec{B} = |\vec{A}| |\vec{B}| \cos \theta_{AB} = 0
\]

Here, the inner product of the \( u_n(x) \) functions is defined over the interval \( a \leq x \leq b \) as:
\[
\langle u_m | u_n \rangle = \int_a^b u_m^*(x) \cdot u_n(x) \, dx
\]

2) The \( u_n(x) \) are **normalized** functions on the interval \( a \leq x \leq b \), i.e. 
\[
\langle u_m | u_n \rangle = \int_a^b u_m^*(x) \cdot u_n(x) \, dx = \int_a^b |u_n(x)|^2 \, dx = 1 \quad \text{(for all } n: \, n = 0, 1, 2, 3, \ldots)\]
\[
|u_n(x)|^2 = u_n^*(x) \cdot u_n(x)
\]

Because the \( u_n(x) \) are **orthonormal** functions, this means that on the interval \( a \leq x \leq b \) :
\[
\langle u_m | u_n \rangle = \int_a^b u_m^*(x) \cdot u_n(x) \, dx = \begin{cases} 0 & \text{if } m \neq n \\ 1 & \text{if } m = n \end{cases}
\]

| \( u_n(x) \) orthogonality on interval \( a \leq x \leq b \) : | \( \int_a^b u_m^*(x) \cdot u_n(x) \, dx = 0 \quad \iff \quad u_m(x) \perp u_n(x) \) |
|---------------------------------------------------------------|
| \( u_n(x) \) normalized on interval \( a \leq x \leq b \) : | \( \int_a^b u_n^*(x) \cdot u_n(x) \, dx = \int_a^b |u_n(x)|^2 \, dx = 1 \) |

We define a mathematical function known as the **Kroenecker \( \delta \)-function**, represented by the symbol, \( \delta_{nm} \) which has the following properties:

<table>
<thead>
<tr>
<th>Kroenecker ( \delta )-function</th>
<th>( \delta_{nm} = 0, \text{ if } n \neq m )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \delta_{nm} = 1, \text{ if } n = m )</td>
</tr>
</tbody>
</table>

Then:
\[
\langle u_m | u_n \rangle \equiv \int_a^b u_m^*(x) \cdot u_n(x) \, dx = \delta_{nm}
\]

on the interval \( a \leq x \leq b \)

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:

\[ \hat{r} = x\hat{x} + y\hat{y} + z\hat{z} \]

\[ |\hat{r}| = \sqrt{x^2 + y^2 + z^2} \]

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

\[ x = \hat{r} \cdot \hat{x} = |\hat{r}| \cos \theta_x \quad (|\hat{x}| = 1) \quad (\cos \theta_x = \hat{r} \cdot \hat{x} = x\text{-direction cosine}) \]

\[ y = \hat{r} \cdot \hat{y} = |\hat{r}| \cos \theta_y \quad (|\hat{y}| = 1) \quad (\cos \theta_y = \hat{r} \cdot \hat{y} = y\text{-direction cosine}) \]

\[ z = \hat{r} \cdot \hat{z} = |\hat{r}| \cos \theta_z \quad (|\hat{z}| = 1) \quad (\cos \theta_z = \hat{r} \cdot \hat{z} = z\text{-direction cosine}) \]

Direction Cosines in 3-D “Real” Space

In Hilbert Space (\( \infty \)-dimensional) the coefficients \( a_n (a_0, a_1, a_2, a_3...) \) (may be real or complex, if \( u_n (x) \) are real or complex) are the projections of \( f(x) = “\text{vector}” \) in Hilbert Space, onto the \( u_n (x) \) orthonormal axis/basis vectors, respectively, i.e.
This means that any 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 $a \leq x \leq b$), we take inner products/dot-products of $u_n(x)$ with $f(x)$:

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

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

$$= \int_a^b u_n^*(x) \left[ a_0 u_0(x) + a_1 u_1(x) + \ldots + a_n u_n(x) + \ldots \right] \, dx$$

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

$$= a_n \int_a^b u_n^*(x) u_n(x) \, dx = a_n \delta_{nk} \quad \left( \delta_{nk} = 0 \text{ if } n \neq k \right) \quad \left( \delta_{nk} = 1 \text{ if } n = k \right)
Let’s consider a real function \( f(x) \) on the real interval \( a \leq x \leq b \). We know that it is possible to exactly represent \( f(x) \), (well-behaved) on the interval \( a \leq x \leq b \) by a power series expansion:

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

because the \( x^n \) polynomials form a complete set on the real, \( \infty \)-dimensional space \( \mathbb{R}^\infty \).

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 \( \infty \)-dimensional Hilbert Space \( \mathbb{R}^\infty \).

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

For example, the Fourier functions (sines & cosines)

\[
\begin{align*}
\sin(nx) &= \frac{x}{1!} - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \ldots = \sum_{k=0, \text{odd}}^{\infty} (-1)^{\frac{k-1}{2}} \frac{x^k}{k!} = \sum_{\ell=1}^{\infty} (-1)^{\ell-1} \frac{x^{2\ell}}{(2\ell-1)!} k = 2\ell - 1 \\
cos(nx) &= \frac{x}{2!} - \frac{x^4}{4!} + \frac{x^6}{6!} + \ldots = \sum_{k=0, \text{even}}^{\infty} (-1)^{\frac{k}{2}} \frac{x^k}{k!} = \sum_{\ell=0}^{\infty} (-1)^{\ell} \frac{x^{2\ell}}{(2\ell)!} k = 2\ell
\end{align*}
\]

where: \( k! = k(k-1)(k-2)\ldots3\cdot2\cdot1 \) and \( 0! = 1, \ 1! = 1, \ 2! = 2, \ 3! = 6, \ \text{etc…} \)

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

We simply/just list these for now:

<table>
<thead>
<tr>
<th>Legendre Functions/Polynomials:</th>
<th>( P_n(x) )</th>
<th>( Q_n(x) ) (singular @ ( x = 0 ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tschebychev Polynomials:</td>
<td>( T_n(x) )</td>
<td>( U_n(x) )</td>
</tr>
<tr>
<td>Jacobi/Elliptic Polynomials:</td>
<td>( K_n(x) )</td>
<td>( K'_n(x) )</td>
</tr>
<tr>
<td>Bessel Functions (1\textsuperscript{st} &amp; 2\textsuperscript{nd} kind):</td>
<td>( J_n(x) )</td>
<td>( N_n(x) )</td>
</tr>
<tr>
<td>Hermite Polynomials:</td>
<td>( H_n(x) )</td>
<td>( H'_n(x) )</td>
</tr>
<tr>
<td>Laguerre Polynomials:</td>
<td>( L_n(x) )</td>
<td>( L'_n(x) )</td>
</tr>
</tbody>
</table>

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 \( \infty \)-dimensional Hilbert Space – to another set of orthonormal basis vectors (e.g. Legendre Polynomials).
Rotations in Real 3-D Space:

\[ \mathbf{r} \text{ expressed in } x\hat{i} + y\hat{j} + z\hat{k} \text{ basis} = \mathbf{r}' \text{ expressed in } x'\hat{i} + y'\hat{j} + z'\hat{k} \text{ basis} \]

\[ x' = x', \ y' = y', \ z' = z' \]

\[ x' - y' - z' \text{ basis is related to } x - y - z \text{ basis by sequence of rotations (e.g. } \varphi \text{ about } \hat{z} \text{ axis, then} \]

\[ \xi \text{ about new } \hat{y} \text{ axis:} \]

\[
\begin{pmatrix}
  x' \\
  y' \\
  z'
\end{pmatrix} =
\begin{pmatrix}
  \text{Rotation Matrix} \\
  \end{pmatrix}
\begin{pmatrix}
  x \\
  y \\
  z
\end{pmatrix}
\]

\[ X' = RX \]

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

\[ f(x) = \sum_{n=0}^{\infty} a_n u_n(x) = \sum_{n=0}^{\infty} b_n u'_n(x) \]