Hilbert Spaces and Gaussian Quadrature (GQ) PhL 1.20.05

Here we first review the Hilbert space H_∞ (L_2 norm), and then we define a new Hilbert space H_N by defining its scalar product. No use of quantum mechanical bra-ket notation appears until after the basics are all established, then we talk bras and kets in items 5 and 6.

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1. The Hilbert Space H_∞. We know that the L2-norm and associated Hilbert space H_∞ can be expressed in terms of a scalar product

$$(f_1, f_2)_\infty = \int dx\, w(x)\, f_1(x)\, f_2(x)$$

where f_1 and f_2 are square-integrable functions (and therefore have finite norms). We know that we can associate with w(x) and interval (a,b) [not shown] a system of orthonormal polys $P_n(x)$ with n = 0,1..∞ and with this **basis** we can associate the following orthogonality and completeness relations:

$(P_n, P_m)_\infty = \delta_{n,m}$	n,m = 0,1,2...∞	orthogonality	H_∞
$\delta(x - x')/w(x) = \Sigma_{n=0}^{\infty} P_n(x)P_n(x')$	x,x' in (a,b)	completeness	

As a check on the completeness relation, we can apply $\int dx\, w(x)\, P_m(x)$ to both sides to get

$$P_m(x') = \int dx\, w(x)\, P_m(x)\Sigma_{n=0}^{\infty} P_n(x)P_n(x') = \Sigma_{n=0}^{\infty} P_n(x')\, (P_n, P_m)_\infty = \Sigma_{n=0}^{\infty} P_n(x')\, \delta_{m,n} = P_m(x')$$

2. GQ for Polys(N-1). We know that for polys(N-1) (polys of degree N-1 or less) we can do GQ which we write as

$$\int dx\, w(x)\, p(x) = \Sigma_{i=1}^{N} A_i\, p(x_i)$$

where p(x) is a poly in Polys(N-1), and we have an N-point GQ. This holds for any choice of $\{ x_i \}$.

3. GQ for Polys(2N-1).If we choose the x_i as zeros of $P_N(x)$, the degree-N ortho poly of the w(x) and (a,b) system, then we know that the above GQ is value for Polys(2N-1). We can then say, for example, that

$$\int dx\, w(x)\, p_1(x)p_2(x) = \Sigma_{i=1}^{N} A_i\, p_1(x_i)p_2(x_i)$$

where p_1 and p_2 are functions in the space Polys(N-1). In this case, $p_1(x)p_2(x)$ is degree 2N-2 which is in fact one less than 2N-1, so we even have room to spare.

4. The Hilbert Space H_N. Item 3 suggests that we might be able to define a new scalar product for functions in Poly(N-1) which are evaluated at the N points x_i as follows

$(p_1, p_2)_N \equiv \Sigma_{i=1}^{N} A_i\, p_1(x_i)p_2(x_i)$ scalar product in H_n H_N

Then we know from item 3 that

$(p_1, p_2)_N = (p_1, p_2)_\infty$

for any p_1, p_2 in Polys(N-1). We can form a basis for Polys(N-1) as $\beta(x) = \{ x^0, x^1, ... x^{N-1} \}$ and therefore this space has dimension N. Of course then the basis for our new space would be $\beta(x_i)$. But we would rather use the basis $\beta'(x_i) = \{ P_0(x_i), P_1(x_i), ... P_{N-1}(x_i) \}$ as we shall show in a moment.

For functions in Polys(N-1), we can "prove" that $(p_1, p_2)_N$ really is a viable scalar product (and therefore we really have a Hilbert Space associated with it) because it is equal, for that range of functions, to something that we know really IS a scalar product, and thus has all the required properties such as linearity. Thus, we know that $(p_1, p_2)_N$ defines a Hilbert space which we will call H_N. We shall call our original infinite Hilbert space H_∞.

What are the orthogonality and completeness relations for H_N ? First, we repeat what they were for H_∞ as was noted earlier

$(P_n, P_m)_\infty = \delta_{n,m}$ $n,m = 0,1,2...\infty$ orthogonality

$\delta(x - x')/w(x) = \Sigma_{n=0}^{\infty} P_n(x)P_n(x')$ x,x' in (a,b) completeness

Then for H_N we have $(P_n, P_m)_N = (P_n, P_m)_\infty = \delta_{n,m}$ from the definition of our H_N scalar product, so we can write these equations for orthogonality and completeness (see note at end regarding orthog sum rule)

$(P_n, P_m)_N = \delta_{n,m}$ $[= \Sigma_{i=1}^{N} A_i\, P_n(x_i)P_m(x_i)\,]$ $n,m = 0,1,2...N-1$ orthogonality H_N

$\delta_{k,j}\,/A_k = \Sigma_{n=0}^{N-1} P_n(x_k)P_n(x_j)$ $i,j = 1...N$ completeness

As a check on the completeness relation, we can apply $\Sigma_{k=1}^{N} A_k\, P_m(x_k)$ to both sides to get

$LHS = \Sigma_{k=1}^{N} A_k\, P_m(x_k)\delta_{k,j}\,/A_k = P_m(x_j)$

$RHS = \Sigma_{k=1}^{N} A_k\, P_m(x_k)\, \Sigma_{n=0}^{N-1} P_n(x_k)P_n(x_j) = \Sigma_{n=0}^{N-1} P_n(x_j)\, \Sigma_{k=1}^{N} A_k\, P_m(x_k)P_n(x_k)$
$= \Sigma_{n=0}^{N-1} P_n(x_j)\, (P_n, P_m)_N = \Sigma_{n=0}^{N-1} P_n(x_j)\, \delta_{n,m} = P_m(x_j)$

You could imagine that within the interval (a,b) we could make the number of points x_i get larger and larger. For finite N we might write the completeness in this manner

$$\Sigma_{n=0}^{N-1} P_n(x_k)P_n(x_j) = \delta_{k,j}/A_k = \text{sinc1}(x_k - x_j)/A(x_k)$$

where sinc1 is some sinc-like function that interpolates the function $\delta_{k,j}$ between the integers. Then in the limit $N\to\infty$, this sinc1 function becomes a delta function, and $A(x_k)$ becomes $w(x)$.

Finally, let's rewrite the completeness relation in its two cases

$0 = \Sigma_{n=0}^{N-1} P_n(x_k)P_n(x_j)$ $\quad k\neq j \quad i,j = 1...N \quad$ completeness $\quad H_N$

$1/A_k = \Sigma_{n=0}^{N-1} [P_n(x_k)]^2$ $\quad k=j \quad i,j = 1...N \quad$ completeness

This last expression gives us a new way to compute the weight for GQ. The formula shown in Scheid requires an integral of the Lagrange multiplier, but here we have a simple sum. We could if we liked use the C-D identity to evaluate the sum. Since our P_n are orthonormal, we have $h_n = 1$ for them (p 159 E),

$1/A_k = \Sigma_{n=0}^{N-1} [P_n(x_k)]^2 = (k_{N-1}/k_N)\, P_{N-1}(x_k)\, P_N'(x_k)$ $\quad$ compute A_k from the polys at x_k

and this is then yet another formula for the GQ weight A_k. Notice that if you do the Jacobi matrix diagonalization procedure, the eigenvalues are the x_k and the eigenvectors are $\mathbf{P}(x_k)$, so you can add up the squares of the elements of the eigenvector $\mathbf{P}(x_k)$ to get $1/A_k$. That seems a good way to compute the Gaussian weights.

5. Bra-ket Notation for H_∞. Let's go back now to our H_∞ Hilbert space discussion where we had

$(P_n, P_m)_\infty = \delta_{n,m}$ $\quad n,m = 0,1,2...\infty \quad$ orthogonality

$\delta(x - x')/w(x) = \Sigma_{n=0}^{\infty} P_n(x)P_n(x')$ $\quad x,x' \text{ in } (a,b) \quad$ completeness

We now give life to a function f independent of its "representation". Normally we think of two representations of a function, coordinate space x and momentum space k (or p), which are related by Fourier transforms. The main idea is to think of a function completely in the abstract as a vector in H_∞ which we write as $| f >$. At the same time we define some vectors $| x >$ which are eigenvectors of the position operator X,

$$X | x > = x | x >$$

We then write the function as $f(x) = <x | f >$. The basis functions can be written as $| P_n >$ or just $| n >$ for short. We might write $F(p) = <p | f >$ in the momentum basis, where now $| p>$ are the eigenvectors of the momentum operator P, similar to our last equation with $x \to p$ everywhere.

Now, the X operator is Hermitian and its eigenvectors $| x>$ therefore form an orthonormal **basis** for H_∞ . We can write orthogonality and completeness in this manner for the $|x>$ basis,

$< x | x' > = \delta(x-x')/w(x)$ $\quad x,x' \text{ in } (a,b) \quad$ orthogonality $\quad H_\infty$

$1_\infty = \int dx\, w(x) | x >< x|$ $\quad$ completeness (this is an "operator" equation)

As a check on this completeness, if we close with <x'| we get

$$<x'|\, 1_\infty = \int dx\, w(x) <x' \mid x><x|\, = <x'|$$

Since this is true for *every* <x'| in H_∞, it must be true in the operator sense shown above.

Alternatively, we could sandwich our P_n basis vectors <n | and | m> around 1_∞ to get

$$<n \mid m> = <n \mid 1_\infty \mid m> = \int dx\, w(x)<n \mid x><x \mid m> = \int dx\, w(x)P_n(x)P_m(x) = (P_n, P_m)_\infty = \delta_{n.m}$$

which is to say

$$<n \mid m> = (P_n, P_m)_\infty = \text{another notation for the } H_\infty \text{ scalar product.}$$

so everything is consistent. This bra-ket notation is useful because it allows us to think of abstract representation-independent operators in a Hilbert space H_∞' which is isomorphic to the space H_∞ whose elements are functions f(x), and then we make no big distinction between H_∞' and H_∞.

Just as the vectors |x> form a basis for H_∞, so do the vectors |m>. Obviously each of these bases has infinite dimension. In the |m> basis we have the following orthogonality and completeness conditions,

$<n \mid m> = \delta_{n.m}$	n,m = 0,1,2...∞	orthogonality	H_∞
$1_\infty = \Sigma_{m=0}^{\infty} \mid m><m \mid$		completeness (operator equation)	

We have already derived the orthogonality in the last paragraph. As a check on completeness, we can close from the left side say with <n | to get the consistent result <n | = <n |. Again, since this is true for every one of the infinite number of basis vectors < n |, the operator equation is true stand alone without projecting onto vectors. We can do the same in the other direction | n > of course.

One can interpret $<n \mid x> = P_n(x)$ as a matrix which changes from one basis to the other.

6. Bra-ket Notation for H_N . We now have N discrete points x_i and our X operator eigenvalue equation is now this

$$X \mid x_i> = x_i \mid x_i>$$

The analogous statements to those of the last section are

$< x_j \mid x_k > = \delta_{j,k}/A_k$	k,j = 1..N	orthogonality	H_N
$1_N = \Sigma_{i=1}^{N} A_i \mid x_i><x_i\mid$	completeness (this is an "operator" equation)		

which we compare to the results in the last section

$< x \mid x' > = \delta(x-x')/w(x)$	x,x' in (a,b)	orthogonality
$1_\infty = \int dx\, w(x) \mid x><x\mid$	completeness (this is an "operator" equation)	

Just as in H_∞ , here the $| x_i >$ form a basis, and the $| m >$ form an alternative basis. Of course here we only have m = 0,1...N-1 instead of up to infinity. Thus, in the $| m>$ basis we have

$<n \mid m> = \delta_{n.m}$ n,m = 0,1,2...N-1 orthogonality H_N

$1_N = \Sigma_{m=0}^{N-1} \mid m >< m \mid$ completeness (operator equation)

which again we compare to the results found for H_∞ ,

$<n \mid m> = \delta_{n.m}$ n,m = 0,1,2...∞ orthogonality

$1_\infty = \Sigma_{m=0}^{\infty} \mid m >< m \mid$ completeness (operator equation)

As before, we can make this identification

$$<n \mid m> = \delta_{n.m} = (P_n, P_m)_N = \Sigma_{i=1}^{N} A_i P_n(x_i) \quad P_m(x_i)$$

We could consider adding a Hilbert Space label to the vectors, so here we would have $|m>_N$ to distinguish it from $|m>_\infty$. For now, I don't think that amount of detail is needed, because we usually know in which space we are working. Sometimes much notation tends to clutter things up and add more confusion rather than less confusion.

Note: We *could* define vectors $| \tilde{x}_i > = (1/\sqrt{A_i}) \mid x_i >$ such that $< \tilde{x}_k \mid \tilde{x}_i > = \delta_{ki}$.

7. The Jacobi Matrix and the E^N space. As an exercise, consider this activity in H_N. Start with

$$X \mid x_i > = x_i \mid x_i >$$

Close from the left with $<n \mid$

$$< n \mid X \mid x_i > = x_i <n \mid x_i >$$

Insert $1_N = \Sigma_{m=0}^{N-1} \mid m >< m \mid$ to the right of operator X,

$$< n \mid X \mid x_i > = < n \mid X\, 1_N \mid x_i > = < n \mid X \Sigma_{m=0}^{N-1} \mid m >< m \mid x_i > = \Sigma_{m=0}^{N-1} < n \mid X \mid m >< m \mid x_i >$$

so we now have this equation

$$\Sigma_{m=0}^{N-1} < n \mid X \mid m >< m \mid x_i > = x_i <n \mid x_i >$$

Now write **$< n \mid X \mid m > = X_{nm}$** in normal matrix notation, and we then have

$$\Sigma_{m=0}^{N-1} X_{nm} P_m(x_i) = x_i P_n(x_i)$$

which in matrix and vector notation we might write as

$X\ \mathbf{P}(x_i) = x_i\mathbf{P}(x_i)$ where $\mathbf{P}(x_i) = \{ P_0(x_i), P_1(x_i), ... P_{N-1}(x_i) \}$ E^N

The matrix X is "the Jacobi matrix" which appears in Jim's papers. That is to say, it is the X operator in the | m > representation. My friend Matthews would write this as $X^{\beta}{}_{\beta}$ where β = the |n> basis.

Now, our matrix X_{nm} is just a normal N x N matrix and as such, it acts on a vector in an E^N space. So now we have another N dimensional space E^N that is not the same as H_N. We don't need a name for this space other than E^N . The scalar product in E^N is the usual E^N one, and is unrelated to the scalar product in H_N.

8. First order perturbation theory. See my doc on this subject. We do this in E^N. We start with

$X\ \mathbf{P}(x_i) = x_i\mathbf{P}(x_i)$

where X is the Jacobi matrix. This is a standard eigenvector equation with a real symmetric matrix X acting on vectors in E^N as noted above. We could just quote the result, but let's do it here anyway:

We do our usual trick by applying a small variation,

$\delta X\ \mathbf{P}(x_i) + X\ \delta\mathbf{P}(x_i) = \delta x_i\ \mathbf{P}(x_i) + x_i\ \delta\mathbf{P}(x_i)$

$\Rightarrow\ \ \delta x_i\ \mathbf{P}(x_i) = \delta X\ \mathbf{P}(x_i) = + [X - x_i 1_N]\ \delta\mathbf{P}(x_i)$

Now close with scalar product in E_N to get

$\delta x_i\ \mathbf{P}(x_i)\bullet\ \mathbf{P}(x_i) = \mathbf{P}(x_i)\bullet\delta X\ \mathbf{P}(x_i) + \mathbf{P}(x_i)\bullet\ [X - x_i 1_N]\ \delta\mathbf{P}(x_i)$

As usual, we use the Hermiticity (real symmetric) of X to rewrite the last term as $\{ [X - x_i 1_N]\mathbf{P}(x_i) \} \bullet \delta\mathbf{P}(x_i) = 0 \bullet \delta\mathbf{P}(x_i) = 0$, and we end up with

$\delta x_i\ \mathbf{P}(x_i)\bullet\ \mathbf{P}(x_i) = \mathbf{P}(x_i)\bullet\delta X\ \mathbf{P}(x_i)$

But we can write

$\mathbf{P}(x_i)\bullet\ \mathbf{P}(x_i) = \Sigma_{m=0}^{N-1} [P_m(x_i)]^2 = 1/A_i \equiv S_i$ // from section 3 above

and we then get our result, as for example in B&B page 5

$\delta x_i = (1/S_i)\ \mathbf{P}(x_i)\bullet[\delta X]\ \mathbf{P}(x_i)$

9. Comments on sum rules and extending GQ from degree N-1 to degree 2N-1

In our item #2 above we talk about GQ for Polys(N-1). I note there that we have

$$\int dx\, w(x)\, p(x) = \Sigma_{i=1}^{N} A_i\, p(x_i) \qquad \text{for any distinct } x_i$$

for p(x) in Polys(N-1). The truth of the above claim is derived as Theorem 1 in my Accuracy of GQ paper. Now we can of course select an Erdelyi ortho poly for p(x) of degree N-1 or less, so we have

$$\int dx\, w(x) p_k(x) = \Sigma_{i=1}^{N} A_i\, p_k(x_i)$$

But then LHS = $(1/k_0) \int dx\, w(x) p_0(x)\, p_k(x) = (h_0/k_0)\, \delta_{k,0}$, so we get our "sum rule"

$$\Sigma_{i=1}^{N} A_i\, p_k(x_i) = (h_0/k_0)\, \delta_{k,0} \qquad k = 0,1,2....N-1 \qquad \text{any distinct } x_i \qquad (1)$$

In the Accuracy of GQ paper, I should how you can use this sum rule and the recursion relation to *extend* the previous sum rule to a larger range of k,

$$\Sigma_{i=1}^{N} A_i\, p_k(x_i) = (h_0/k_0)\, \delta_{k,0} \qquad k = 0,1,2....2N-1 \qquad \text{if } p_N(x_i) = 0 \qquad (2)$$

This then used to show that GQ is good for Polys(2N-1).

Now, once we know this, we go ahead as above and develop the H_N space. We then found that

$$(P_n, P_m)_N = \delta_{n,m} \quad [= \Sigma_{i=1}^{N} A_i\, P_n(x_i) P_m(x_i)\,] \qquad n,m = 0,1,2...N-1 \qquad \text{orthogonality}$$

This provides a generalization of my first sum rule above:

$$\Sigma_{i=1}^{N} A_i\, p_n(x_i) p_m(x_i) = \delta_{n,m} \qquad (3)$$

If I set n = 0 in (3), we get (1).