# Orthogonal Polynomials and Applications to Differential Equations

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# Orthogonal Vectors

When using vectors we usually work with a N-dimensional orthonormal basis and represent the vectors in our space as linear combinations of these basis vectors. For instance in 3 dimensions we have,

$$\vec{V} = V_x\hat{\imath} + V_y\hat{\jmath} + V_z\hat{k}$$

Where the vectors $\hat{\imath}$,$\hat{\jmath}$, and $\hat{k}$ are normalized and orthogonal.

# Orthogonal Vectors

If we want the x-component of $\vec{V}$ we can take advantage of the orthogonality of the basis vectors.

$$\vec{V} \cdot \hat{\imath} = V_x \hat{\imath} \cdot \hat{\imath} + V_y \hat{\jmath} \cdot \hat{\imath} + V_z \hat{k} \cdot \hat{\imath}$$

$$= V_x(1) + V_y(0) + V_z(0)$$

$$= V_x$$

We can get any component of $\vec{V}$ by evaluating its dot product with the appropriate basis vector.

# Orthogonal Polynomials

Two polynomials are orthogonal on an interval $[a, b]$ with respect to the weight function $w(x)$ if,

$$\int_a^b P_1(x)P_2(x)w(x)dx = \begin{cases} 1 \text{ if } P_1 = P_2 \\ 0 \text{ if } P1 \neq P2 \end{cases}$$

If we have a collection of polynomials with this property then we say that they are mutually orthogonal. It is useful to think of this integration as being analogous to a dot product between two vectors. We call this integration the inner product of two functions.

$$\int_a^b f(x)g(x)dx \equiv \langle f|g \rangle$$

# Complete Basis of Polynomials

We can use orthogonal polynomials in the same way that we use the basis vectors $\hat{\imath}, \hat{\jmath}$, and $\hat{k}$.

Any sqaure integrable function on an interval can be written as a linear combination of polynomials times the square root of some appropriate weight function.

$$\int_a^b |f(x)|^2 dx = 1$$

$$\Rightarrow f(x) = \sum_n c_n P_n(x) \sqrt{w(x)}$$

When we do this we can think of $f(x)$ as a collumn vector with components $\{c_n\}$

To make the notation cleaner we usually write,

$$P_n \sqrt{w(x)} \equiv |n\rangle$$

# Fourier's Trick

Recall that to get the components of $\vec{V}$ all we have to do is evaluate the dot product with the appropriate basis vector. This hinged on the orthogonality of the basis vectors. We can use the same trick with orthogonal polynomials to get the coefficients in the superposition.

$$\langle n|f\rangle = \langle n| \sum_m c_m |m\rangle$$

$$= \sum_m c_m \langle n|m\rangle$$

$$= \sum_m c_m \int_a^b P_n(x)P_m(x)w(x)dx$$

$$= \sum_m c_m \delta_{n,m}$$

$$= c_n$$

This is sometimes called Fourier's trick.

# Example : Hermite Polynomials

The hermite polynomials are an example of a complete set of orthogonal polynomials.

$$H_0 = 1, H_1 = 2x, H_2 = 4x^2 - 2, ..., H_n = (-1)^n e^{x^2} \left(\frac{d}{dx}\right)^n e^{-x^2}$$

They have the weight function $w(x) = e^{-x^2}$ and obey the orthogonality condition,

$$\int_{-\infty}^{\infty} H_n H_m e^{-x^2} dx = \begin{cases} 2^n n! \sqrt{\pi} & n = m \\ 0 \quad n \neq m \end{cases}$$

We can normalize these polynomials by dividing them by $2^n n! sqrt \pi$
Then we define,

$$|n\rangle = \frac{1}{\sqrt{2^n n! \sqrt{pi}}} H_n e^{-x^2/2},$$

# Example : Hermite Polynomials

The Hermite polynomial basis is complete so any square integrable function can be written as a superposition of these functions.

$$f(x) = \sum_n c_n |n\rangle$$

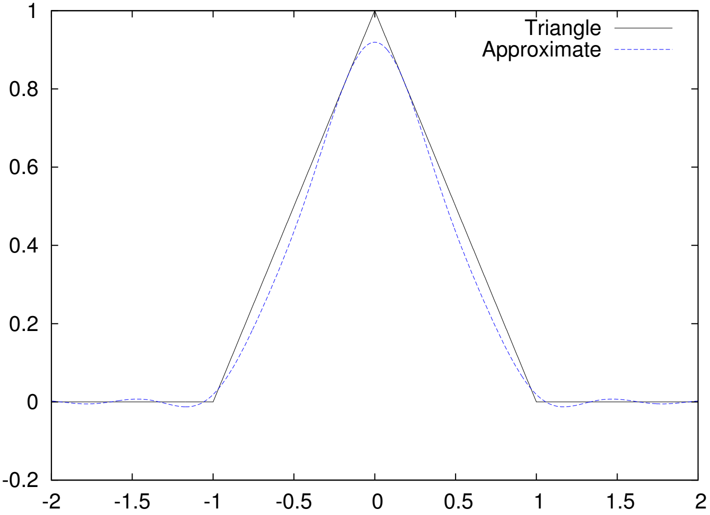
For instance we can expand the following function in this basis.

$$f(x) = \begin{cases} 0 & |x| > 1 \\ 1 + x & -1 \leq x \leq 0 \\ 1 - x & 0 \leq x \leq 1 \end{cases}$$

We get the coefficients by evaluating the integrals,

$$c_n = \langle n|f\rangle = \int_{-\infty}^{\infty} \frac{H_n}{\sqrt{2^n n! \sqrt{\pi}}} e^{-x^2/2} f(x) dx$$

# Approximation of Triangle Function



# Linear Differential Equations

Certain linear differential equations can be turned into matrix equations using orthogonal polynomials. For example consider the Schrödinger equation,

$$-\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = E\psi$$

The differential operator acting on the function $\psi$ is linear,

$$\hat{H} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x)$$

$$\hat{H}\left(f(x) + g(x)\right) = \hat{H}f(x) + \hat{H}g(x)$$

# Differentail Equations as a Matrix Eigenvalue Problem

We know that any square integrable function can be written as the superposition of some complete basis.

$$\psi(x) = \sum_n c_n |n\rangle$$

If we apply our differential operator $\hat{H}$ to this function we get,

$$\hat{H}\psi(x) = \hat{H}\sum_n c_n |n\rangle$$

Because operator is linear we can distribute it through the sum,

$$\hat{H}\psi(x) = \sum_n c_n \hat{H} |n\rangle$$

# Differentail Equations as a Matrix Eigenvalue Problem

If $\psi$ solves the Schrödinger equation then we can write,

$$\hat{H}\psi = E\psi$$

$$\sum_n c_n \hat{H} \left| n \right\rangle = E \sum_n c_n \left| n \right\rangle$$

Now we take the inner product of both sides with the basis vector $\left| m \right\rangle$

$$\sum_n c_n \left\langle m \right| \hat{H} \left| n \right\rangle = E \sum_n c_n \left\langle m | n \right\rangle$$

$$\sum_n c_n H_{mn} = E \sum_n c_n \delta_{mn}$$

$$\sum_n c_n H_{mn} = E c_m$$

# Differentail Equations as a Matrix Eigenvalue Problem

The expression on the right of the equation below is the multiplication of a matrix $H_{mn}$ with a column vector $c_n$. Since the result of this multiplication is a constant times the original vector we have a matrix eigenvalue problem.

$$\sum_n c_n H_{mn} = E c_m$$

$$\begin{pmatrix} H_{00} & H_{01} & H_{02} & \cdots \\ H_{10} & H_{11} & H_{13} & \cdots \\ H_{20} & H_{21} & H_{22} & \cdots \\ H_{30} & H_{31} & H_{32} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix} = E \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}$$

If we were lucky enough to choose a basis that makes $H_{nm}$ diagonal then the functions of that basis would solve this equation.

# References


- William H. Press, Saul A. Teukolsky, William T. Vetterling, Brian P. Flannery, *Fortran Numerical Recipes*. Cambridge University Press, New York, 2nd Edition, 1996.
- Milton Abromowitz, Irene A. Stegun, *Handbook of Mathematical Functions With Formulas, Graphs, and Mathematical Tables*. National Bureau of Standards Applied Mathematics Series, 1972.
- Bryant, Brandon Charls, "Lagrange Meshes in Hardronic Physics" (2011). *Honors Theses*. Paper 6. http://diginole.lib.fsu.edu/uhm/6
- Baye, D. (2006), Lagrange-mesh method for quantum-mechanical problems. Phys. Status Solidi B, 243: 1095-1109. doi: 10.1002/pssb.200541305