

Orthogonality and Computation

Daniel Topa

HPCMPO PETTT Engility Corp. ERDC DSRC Vicksburg MS

Thursday 21st January, 2016

Problem statement

Paean to orthogonality Lebesgue spaces Computation in ℓ^2 Validation

Orthogonal functions Summation



Overview

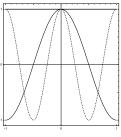


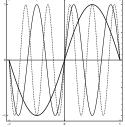


- sines and cosines
- Bessel functions
- Laguerre polynomials
- 4 Hermite polynomials
- Ohebyshev polynomials
- Legendre polynomials
- Jacobi polynomials
- 6 Gegenbauer polynomials
- Zernike polynomials
- Spherical harmonics



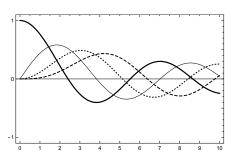
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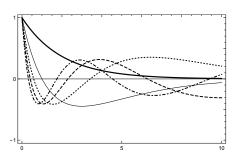


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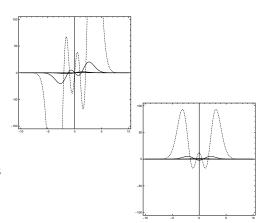


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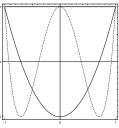


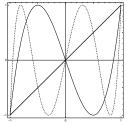
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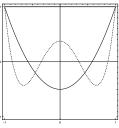
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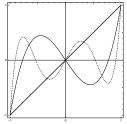






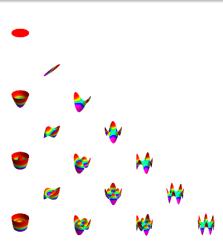
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Orthogonal functions

Popular functions orthogonal in computation

- sines and cosines
- Bessel functions
- 4 Hermite polynomials
- 6 Chebyshev polynomials
- 6 Legendre polynomials
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Critical observation

The only functions orthogonal in the continuum and in discrete space:

 $\sin nx$, $\cos nx$



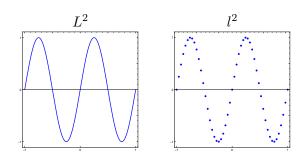
Rudiments

Orthogonality depends upon

- domain
- topology (continuous or discrete)



Snapshot



 L^2 is not l^2

That's why they have different symbols



Prototype linear equation

$$\mathbf{A}x = b$$

$$x_1 \begin{bmatrix} a_{11} \\ \vdots \\ a_{m1} \end{bmatrix} + \dots + x_n \begin{bmatrix} a_{1n} \\ \vdots \\ a_{mn} \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix}$$

Problem statement
Paean to orthogonality
Lebesgue spaces
Computation in l^2 Validation

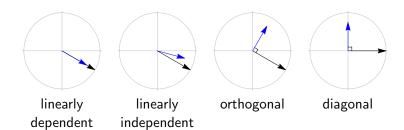
Linear Systems General case Diagonal matrices



Condition Number

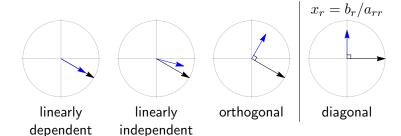


Column vectors of A





Column vectors of A: clicks





Column vectors of $A: L^2$

Linearly Independent

Orthogonal

Diagonal Laguerre

Zernike Jacobi trigonometric Legendre Spherical harmonics Gegenbauer Hermite Chebyshev Bessel



Column vectors of $A: l^2$

Linearly Independent

Zernike
Jacobi
Gegenbauer
Legendre
Hermite
Bessel
Chebyshev
Laguerre
Spherical harmonics

Orthogonal

Diagonal trigonometric



General System

$$\mathbf{A}x = b$$

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}^{-1} \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$



Diagonal System

$$\mathbf{A}x = b$$

$$\begin{bmatrix} \alpha_1 & 0 \\ 0 & \alpha_2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

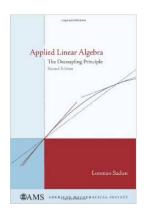
$$\left[\begin{array}{c} x_1 \\ x_2 \end{array}\right] = \left[\begin{array}{cc} 1/\alpha_1 & 0 \\ 0 & 1/\alpha_2 \end{array}\right] \left[\begin{array}{c} b_1 \\ b_2 \end{array}\right]$$



Decoupling Principle

Diagonal Systems are decoupled

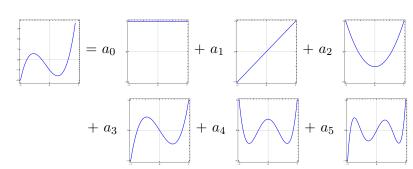
- difference equations
- Markov chains
- coupled oscillators
- Fourier series
- wave equation
- Schrodinger equation





L^2 : Legendre Basis

$$F(x) \approx \sum_{k=0}^{d} a_k P_k(x)$$





l^2 : Legendre Basis

$$f(x) \approx \sum_{k=0}^{d} b_k P_k(x)$$

$$= b_0 + b_1 + b_2 + b_2 + b_3 + b_4 + b_5 + b_5$$



Finding the Amplitudes

Finding amplitudes = Solving linear systems



Formalities

Orthogonality and Computation



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Abstract—The property of orthogonality is predicated upon the specifications of a domain and a topology. The orthogonality of the continuum is violated in the computational domain as evidenced by poor convergence and numerical oscillations. Penalties are significant numerical errors and a substantial increase in computation time. By using linear independence, exact solutions are found in specific instances.

Keywords: orthogonality, linear independence, Hilbert space, Lebesgue integration, domain topology

1. Introduction

Orthogonality and projection are two facets of the same gem. They are foundation concepts in many areas of science and engineering. For example, the mathematics of quantum mechanics and quantum field theory are the embodiment of the power of orthogonal projection. The least squares method that it gives rise to the so-called Sobolev spaces, where the smoothness of the function f(x) is understood in terms of the L^2 -norm, and the corresponding decay of the coefficients is given in the related l^2 -norm via

$$\int_{-\pi}^{\pi} \left| \frac{d^k f}{dx^k} \right|^2 dx = \sum_{n=-\infty}^{n=\infty} n^{2k} |c_n|^2. \quad (1.1)$$

The spaces L^2 and ℓ^2 are distinct and, excluding sine and cosine, there are no functions which are orthogonal in both.

2. Spaces and Topologies

Troubles arise when moving from the continuous space L^2 to the discrete space of l^2 . This corresponds to moving from the continuum, the theoretical realm of the chalkboard, to discrete space, the realm of computer calculation. Either measurement or computation imply a discrete topology which sacrifices orthogonality.



Normal Equations: General Case

	system	sol'n	data
L^2 :	$\begin{bmatrix} \langle G_0 G_0\rangle & \langle G_0 G_1\rangle & \cdots & \langle G_0 G_d\rangle \\ \langle G_1 G_0\rangle & \langle G_1 G_1\rangle & \cdots & \langle G_1 G_d\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle G_d G_0\rangle & \langle G_d G_1\rangle & \cdots & \langle G_d G_d\rangle \end{bmatrix}$	$\left[\begin{array}{c} a_0 \\ a_1 \\ \vdots \\ a_d \end{array}\right] = $	$\begin{bmatrix} \langle F G_0 \rangle \\ \langle F G_1 \rangle \\ \vdots \\ \langle F G_d \rangle \end{bmatrix}$
l^2 :	$\begin{bmatrix} \langle g_0 g_0\rangle & \langle g_0 g_1\rangle & \cdots & \langle g_0 g_d\rangle \\ \langle g_1 g_0\rangle & \langle g_1 g_1\rangle & \cdots & \langle g_1 g_d\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle g_d g_0\rangle & \langle g_d g_1\rangle & \cdots & \langle g_d g_d\rangle \end{bmatrix}$	$\left[\begin{array}{c}b_0\\b_1\\\vdots\\b_d\end{array}\right]=$	$\begin{bmatrix} \langle f g_0\rangle \\ \langle f g_1\rangle \\ \vdots \\ \langle f g_d\rangle \end{bmatrix}$



Expression of Orthogonality

$$m \neq n$$

$$L^2$$
: $\langle G_m | G_n \rangle = \int_{\Omega} G_m(x) G_n(x) dx = 0$

$$l^2$$
: $\langle g_m | g_n \rangle = \sum_{x \in \sigma} g_m(x) g_n(x) \Delta =$

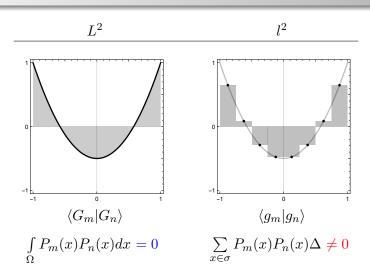


Normal Equations: Orthogonal Basis

		system		sol'n	data
L^2 :	$\begin{bmatrix} \langle G_0 G_0 \rangle \\ 0 & \langle 0 \\ \vdots \\ 0 \end{bmatrix}$	$egin{array}{ccc} 0 & \cdots \ G_1 G_1 angle & \cdots \ \vdots & \cdots \ 0 & \cdots \end{array}$	0	$\left[\begin{array}{c} a_0 \\ a_1 \\ \vdots \\ a_d \end{array}\right] = $	$\begin{bmatrix} \langle F G_0 \rangle \\ \langle F G_1 \rangle \\ \vdots \\ \langle F G_d \rangle \end{bmatrix}$
l^2 :	$\left[egin{array}{c} \langle g_0 g_0 angle \ 0 \ dots \ 0 \end{array} ight.$	$\begin{pmatrix} 0 & \cdots \\ \langle g_1 g_1 \rangle & \cdots \\ \vdots & \ddots \\ 0 & \cdots \end{pmatrix}$		$\left[\begin{array}{c}b_0\\b_1\\\vdots\\b_d\end{array}\right]=$	$\begin{bmatrix} \langle f g_0 \rangle \\ \langle f g_1 \rangle \\ \vdots \\ \langle f g_d \rangle \end{bmatrix}$



In a Nutshell

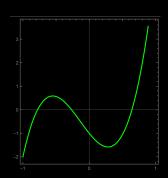


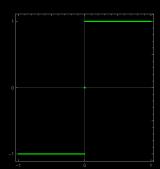
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Examples
Continuous function
Discontinuous Functior
Solutions



Smoothness







Monomials and Legendre Polynomials

k	$M_k(x)$	$P_k(x)$
0	1	1
1	\boldsymbol{x}	x
2	x^2	$\frac{1}{2}\left(3x^2-1\right)$
3	x^3	$rac{1}{2}\left(5x^3-3x ight)$
4	x^4	$\frac{1}{8}\left(35x^4 - 30x^2 + 3\right)$
5	x^5	$\frac{1}{8}\left(63x^5 - 70x^3 + 15x\right)$
6	x^6	$\frac{1}{16} \left(231x^6 - 315x^4 + 105x^2 - 5 \right)$
7	x^7	$\frac{1}{16} \left(429x^7 - 693x^5 + 315x^3 - 35x \right)$
8	x^8	$\frac{1}{128} \left(6435x^8 - 12012x^6 + 6930x^4 - 1260x^2 + 35 \right)$
9	x^9	$\frac{1}{128} \left(12155 x^9 - 25740 x^7 + 18018 x^5 - 4620 x^3 + 315 x \right)$
10	x^{10}	$\frac{1}{256} \left(46189x^{10} - 109395x^8 + 90090x^6 - 30030x^4 + 3465x^2 - 63 \right)$

Examples
Continuous function
Discontinuous Function
Solutions



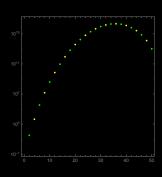
Comparing methods

	faux orthogonality	linear independence
mesh points	10^9	9
error	10^{-9}	0



Degree of fit = 50

amplitudes



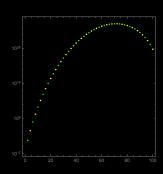
approximation



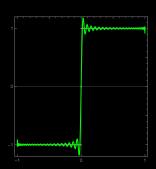


Degree of fit = 100

amplitudes



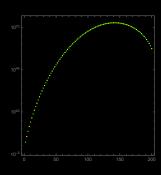
approximation



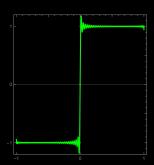


Degree of fit = 200

amplitudes



approximation



Examples
Continuous function
Discontinuous Functio
Solutions



Computing in l^2

Lessons learned

- Both solutions used linear independence, not orthogonality
- Well-conditioned problems allow monomials
- Ill-conditioned problems require Legendre polynomials

Solutions



Off-diagonal entries persist in l^2

Linearly independent system

$$\begin{bmatrix} \langle g_0|g_0\rangle & \langle g_0|g_1\rangle & \cdots & \langle g_0|g_d\rangle \\ \langle g_1|g_0\rangle & \langle g_1|g_1\rangle & \cdots & \langle g_1|g_d\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle g_d|g_0\rangle & \langle g_d|g_1\rangle & \cdots & \langle g_d|g_d\rangle \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_d \end{bmatrix} = \begin{bmatrix} \langle f|g_0\rangle \\ \langle f|g_1\rangle \\ \vdots \\ \langle f|g_d\rangle \end{bmatrix}$$

$$\begin{bmatrix} \langle g_0|g_0\rangle & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \langle g_1|g_1\rangle & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \langle g_d|g_d\rangle \end{bmatrix}$$

$$\begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_d \end{bmatrix} = \begin{bmatrix} \langle f|g_0 \rangle \\ \langle f|g_1 \rangle \\ \vdots \\ \langle f|g_d \rangle \end{bmatrix}$$

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Example Mathematica Spreadsheet Conclusion



Quick Validation

Quick validation uncovers the loss of orthogonality.



Validation Tools

- Simple construction
- Simple interpretation
- Oisplay differences



Simple Example

Define

$$f(x) = 0P_0 + 1P_1(x) + 2P_2(x) + 3P_3(x) + 0P_4 + \dots$$

Compute

$$f(x) \approx b_0 P_0(x) + b_1 P_1(x) + b_2 P_2(x) + b_3 P_3(x) + b_4 P_4(x) + \dots$$

Expectation

$$b_0 = 0$$
, $b_1 = 1$, $b_2 = 2$, $b_3 = 3$, $b_4 = b_5 = b_6 = 0$



Solution vector

$$b_0 = 0$$
, $b_1 = 1$, $b_2 = 2$, $b_3 = 3$, $b_4 = b_5 = b_6 = 0$
$$b = \{0, 1, 2, 3, 0, 0, 0\}$$



Function and Mesh

solve for amplitudes

input function

$$\begin{aligned} &\text{mesh} &f[\textbf{x}] = \text{LegendreP[1, x] + 2 LegendreP[2, x] + 3 LegendreP[3, x];} \\ &f(x) = P_1(x) + 2P_2(x) + 3P_3(x) \end{aligned}$$

$$\ln[232] = \Delta = \frac{1}{4};$$

$$\text{mesh} = \text{Range}[-1, 1, \Delta]$$

$$\text{Out}[233] = \left\{-1, -\frac{3}{4}, -\frac{1}{2}, -\frac{1}{4}, 0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1\right\}$$



Linear System and Solution

linear system

```
In[52]:= d = 6; (* order of fit *)
In[53]:= A = Table[
         LegendreP[row, mesh].LegendreP[col, mesh]
          , {row, 0, d}, {col, 0, d}];
      y = Table[
          f[mesh].LegendreP[row, mesh]
          , {row, 0, d}];
   solution
In[55]:= btrue = Inverse[A].y
Out[55]= \{0, 1, 2, 3, 0, 0, 0\}
```



Linear System and Solution

```
 \begin{array}{l} \text{linear system} & \mathbf{A} = \\ & \int P_0(x)P_0(x)dx & \cdots & \int P_0(x)P_d(x)dx \\ & \vdots & \ddots & \vdots \\ & \int P_d(x)P_0(x)dx & \cdots & \int P_d(x)P_d(x)dx \\ & \vdots & \ddots & \vdots \\ & \int P_d(x)P_0(x)dx & \cdots & \int P_d(x)P_d(x)dx \\ & \\ & \text{LegendreP[row, mesh] . LegendreP[col, mesh]} \\ & & , \{\text{row, 0, d}\}, \{\text{col, 0, d}\}; \\ & \mathbf{y} = \mathbf{Table[} \\ & & \mathbf{f[mesh] . LegendreP[row, mesh]} \quad y = \begin{bmatrix} \int f(x)P_0(x)dx \\ & \vdots \\ & \int f(x)P_d(x)dx \end{bmatrix} \\ & & \vdots \\ & \int f(x)P_d(x)dx \end{bmatrix}
```

solution

$$b = \mathbf{A}^{-1}y$$



Misapplication of L^2 Rules

faux-thogonality

```
 \begin{split} & \ln[47] = \text{ bfaux} = \text{Table} \Big[ \\ & \left\{ k \,,\, \frac{2\,k+1}{2}\,\, f\, [\text{mesh}] \,. \text{LegendreP} [\,k \,,\, \text{mesh}] \,\Delta \right\} \\ & \quad , \, \left\{ k \,,\, 0 \,,\, 6 \,\right\} \Big]; \\ & \quad \% \,//\,\, N \\ & \text{Out}[48] = \, \left\{ \{0 \,,\, 0 \,.\, 28125 \} \,,\, \{1 \,,\, 2 \,.\, 85645 \} \,,\, \{2 \,,\, 3 \,.\, 55957 \} \,,\, \{3 \,,\, 8 \,.\, 00125 \} \,,\, \{4 \,,\, 3 \,.\, 41084 \} \,,\, \{5 \,,\, 9 \,.\, 47403 \} \,,\, \{6 \,,\, 6 \,.\, 05371 \} \right\} \\ \end{split}
```



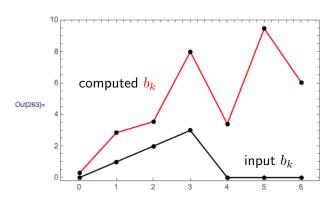
Misapplication of L^2 Rules

faux-thogonality

```
\begin{array}{l} & \text{ln[47]:= bfaux = Table} \left[ \\ & \left\{ \textbf{k}, \left( \frac{\textbf{2 k + 1}}{\textbf{2}} \text{ f[mesh].LegendreP[k, mesh]} \Delta \right) \right. \\ & b_k = \frac{\int_{-1}^1 f(x) P_k(x) dx}{\int_{-1}^1 P_k^* P_k(x) dx} \\ & \text{, } \left\{ \textbf{k}, \textbf{0}, \textbf{6} \right\} \right]; \\ & \textbf{\% // N} \\ & \text{Out[48]:= } \left\{ \{ \textbf{0., 0.28125} \}, \, \{ \textbf{1., 2.85645} \}, \, \{ \textbf{2., 3.55957} \}, \\ & \{ \textbf{3., 8.00125} \}, \, \{ \textbf{4., 3.41084} \}, \, \{ \textbf{5., 9.47403} \}, \, \{ \textbf{6., 6.05371} \} \right. \end{array}
```

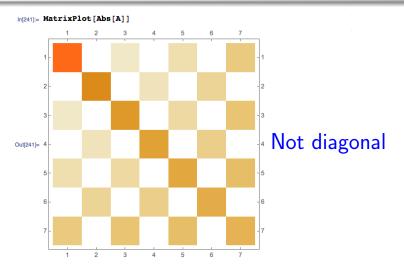


Misapplication of L^2 Rules



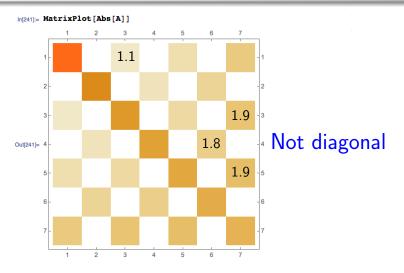


Telling the Story with One Plot



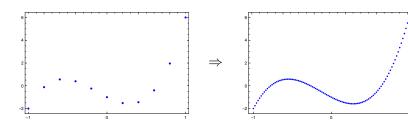


Telling the Story with One Plot



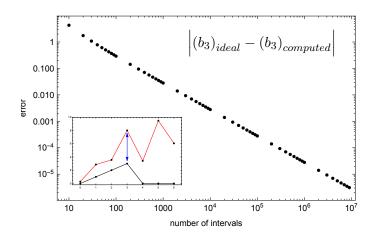


Convergence: shrink interval



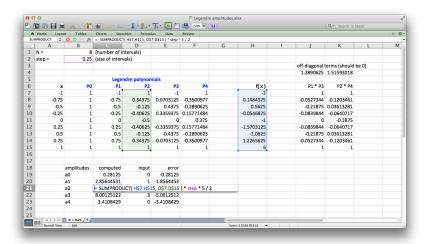


Convergence



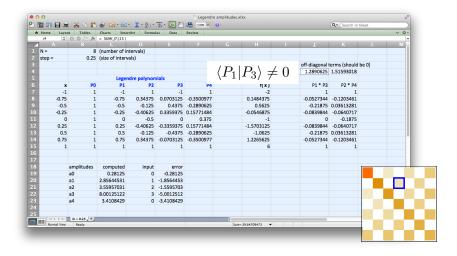


Spreadsheet validation



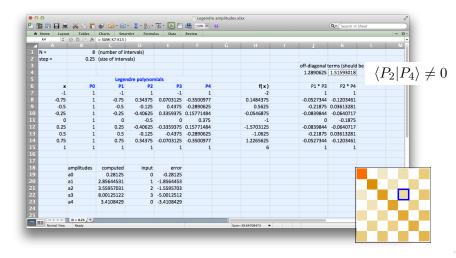


Spreadsheet validation





Spreadsheet validation





Validation Results

- Simple tools uncover problem
- Better tools point to solution



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