

Orthogonality and Computation

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Overview



Orthogonal functions

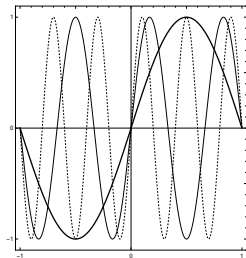
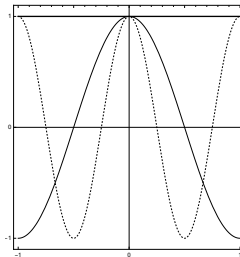
Popular orthogonal functions

- ① sines and cosines
- ② Bessel functions
- ③ Laguerre polynomials
- ④ Hermite polynomials
- ⑤ Chebyshev polynomials
- ⑥ Legendre polynomials
- ⑦ Jacobi polynomials
- ⑧ Gegenbauer polynomials
- ⑨ Zernike polynomials
- ⑩ Spherical harmonics

Orthogonal functions

Popular orthogonal functions

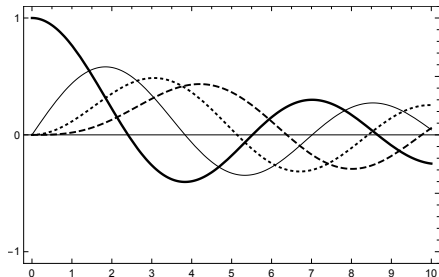
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Orthogonal functions

Popular orthogonal functions

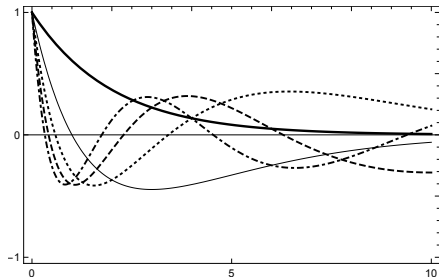
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Orthogonal functions

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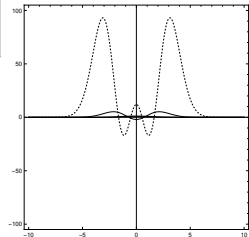
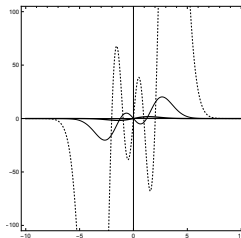
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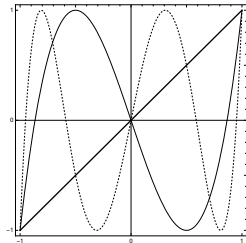
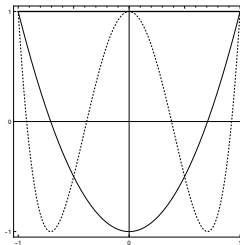
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Orthogonal functions

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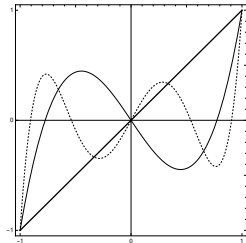
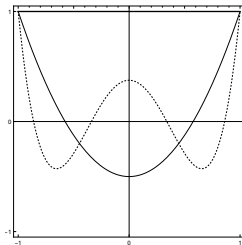
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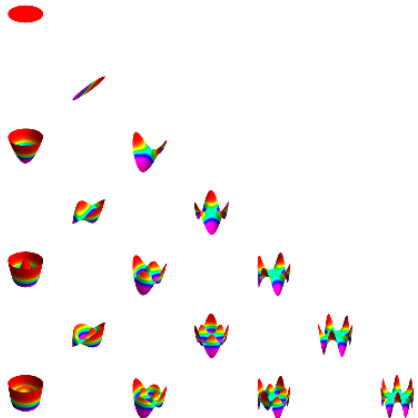
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Orthogonal functions

Popular functions orthogonal in computation

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Critical observation

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

$$\sin nx, \quad \cos nx$$

Rudiments

Orthogonality depends upon

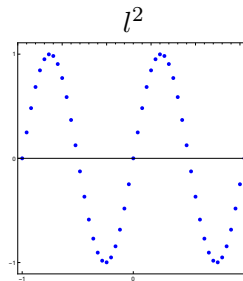
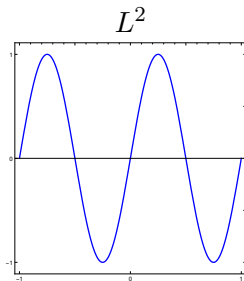
- 1 domain
- 2 topology

Rudiments

Orthogonality depends upon

- ① domain
- ② topology (continuous or discrete)

Snapshot



L^2 is not l^2

That's why they have different symbols

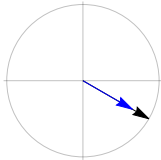
Prototype linear equation

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

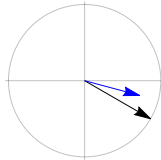
$$x_1 \begin{bmatrix} a_{11} \\ \vdots \\ a_{m1} \end{bmatrix} + \cdots + x_n \begin{bmatrix} a_{1n} \\ \vdots \\ a_{mn} \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix}$$

Condition Number

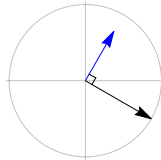
Column vectors of A



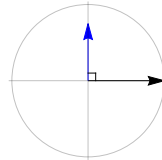
linearly
dependent



linearly
independent

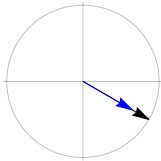


orthogonal

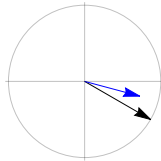


diagonal

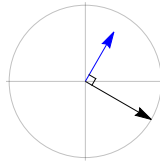
Column vectors of \mathbf{A} : clicks



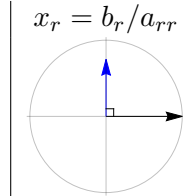
linearly
dependent



linearly
independent

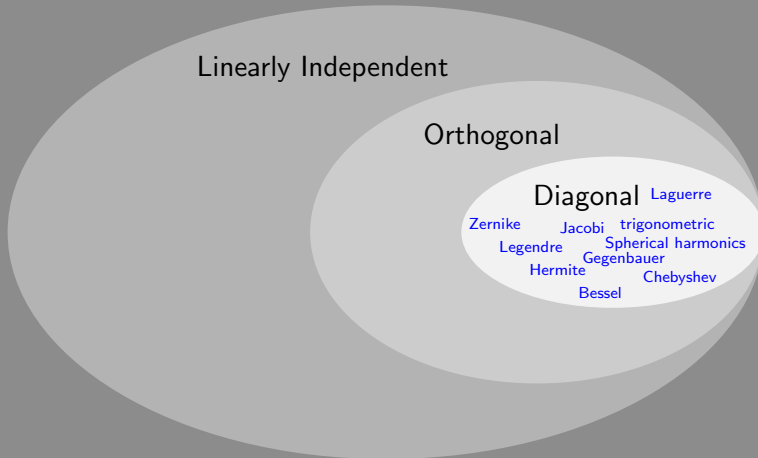


orthogonal

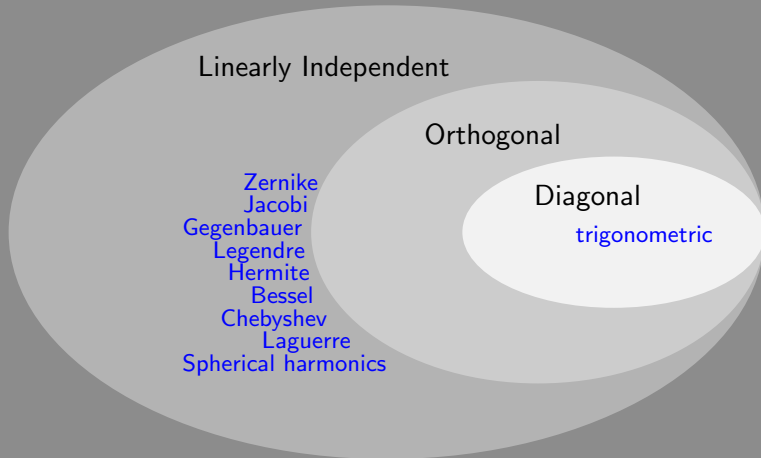


diagonal

Column vectors of \mathbf{A} : L^2



Column vectors of \mathbf{A} : l^2



General System

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

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

\Downarrow

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

Diagonal System

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

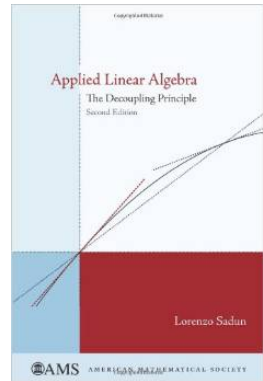
$$\begin{bmatrix} \alpha_1 & 0 \\ 0 & \alpha_2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

\Downarrow

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1/\alpha_1 & 0 \\ 0 & 1/\alpha_2 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

Decoupling Principle

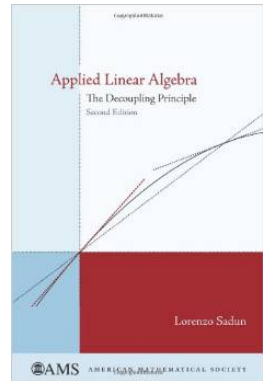
Diagonal Systems are decoupled



Decoupling Principle

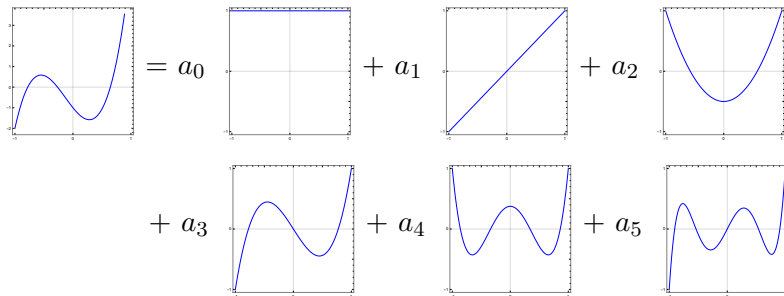
Diagonal Systems are decoupled

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



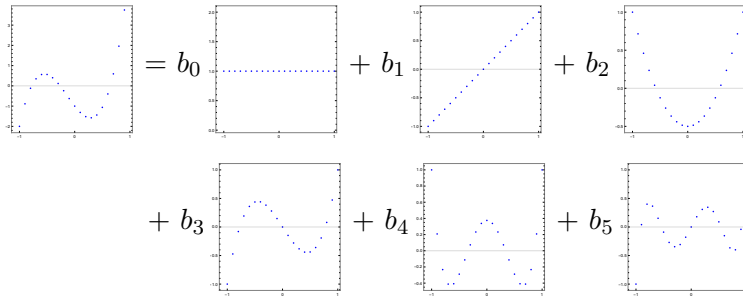
L^2 : Legendre Basis

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



l^2 : Legendre Basis

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



Finding the Amplitudes

Finding amplitudes = Solving linear systems

Formalities

Orthogonality and Computation



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Information Technology Laboratory, Vicksburg MS, USA

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 :	$\begin{bmatrix} \langle G_0 G_0 \rangle & \langle G_0 G_1 \rangle & \cdots & \langle G_0 G_d \rangle \\ \langle G_1 G_0 \rangle & \langle G_1 G_1 \rangle & \cdots & \langle G_1 G_d \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle G_d G_0 \rangle & \langle G_d G_1 \rangle & \cdots & \langle G_d G_d \rangle \end{bmatrix}$		$\begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_d \end{bmatrix}$	=	$\begin{bmatrix} \langle F G_0 \rangle \\ \langle F G_1 \rangle \\ \vdots \\ \langle F G_d \rangle \end{bmatrix}$
l^2 :	$\begin{bmatrix} \langle g_0 g_0 \rangle & \langle g_0 g_1 \rangle & \cdots & \langle g_0 g_d \rangle \\ \langle g_1 g_0 \rangle & \langle g_1 g_1 \rangle & \cdots & \langle g_1 g_d \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle g_d g_0 \rangle & \langle g_d g_1 \rangle & \cdots & \langle g_d g_d \rangle \end{bmatrix}$		$\begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_d \end{bmatrix}$	=	$\begin{bmatrix} \langle f g_0 \rangle \\ \langle f g_1 \rangle \\ \vdots \\ \langle f g_d \rangle \end{bmatrix}$

Expression of Orthogonality

$$m \neq n$$

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

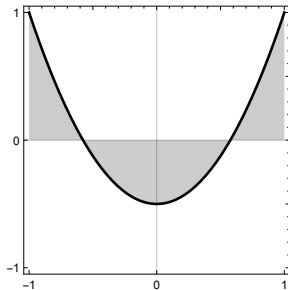
$$l^2: \quad \langle g_m | g_n \rangle = \sum_{x \in \sigma} g_m(x) g_n(x) \Delta = 0$$

Normal Equations: Orthogonal Basis

	system		sol'n		data
$L^2:$	$\begin{bmatrix} \langle G_0 G_0 \rangle & 0 & \cdots & 0 \\ 0 & \langle G_1 G_1 \rangle & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \langle G_d G_d \rangle \end{bmatrix}$		$\begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_d \end{bmatrix}$	=	$\begin{bmatrix} \langle F G_0 \rangle \\ \langle F G_1 \rangle \\ \vdots \\ \langle F G_d \rangle \end{bmatrix}$
$l^2:$	$\begin{bmatrix} \langle g_0 g_0 \rangle & 0 & \cdots & 0 \\ 0 & \langle g_1 g_1 \rangle & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \langle g_d g_d \rangle \end{bmatrix}$		$\begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_d \end{bmatrix}$	=	$\begin{bmatrix} \langle f g_0 \rangle \\ \langle f g_1 \rangle \\ \vdots \\ \langle f g_d \rangle \end{bmatrix}$

In a Nutshell

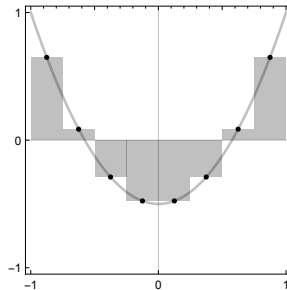
L^2



$\langle G_m | G_n \rangle$

$$\int_{\Omega} P_m(x) P_n(x) dx = 0$$

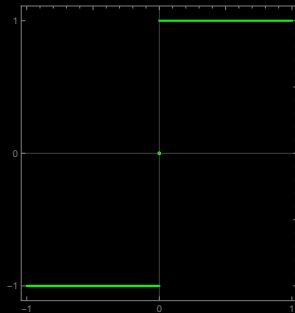
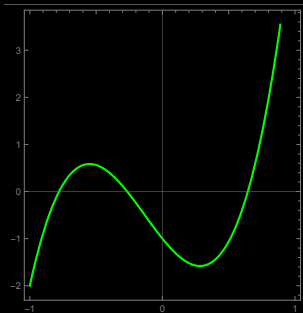
l^2



$\langle g_m | g_n \rangle$

$$\sum_{x \in \sigma} P_m(x) P_n(x) \Delta \neq 0$$

Smoothness

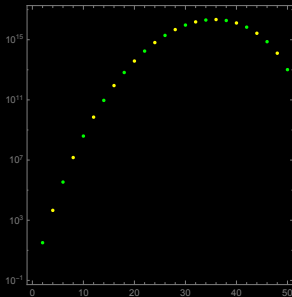


Monomials and Legendre Polynomials

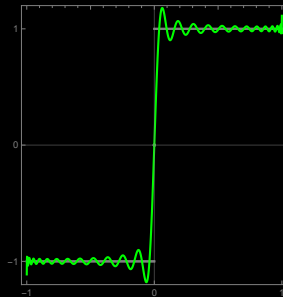
k	$M_k(x)$	$P_k(x)$
0	1	1
1	x	x
2	x^2	$\frac{1}{2} (3x^2 - 1)$
3	x^3	$\frac{1}{2} (5x^3 - 3x)$
4	x^4	$\frac{1}{8} (35x^4 - 30x^2 + 3)$
5	x^5	$\frac{1}{8} (63x^5 - 70x^3 + 15x)$
6	x^6	$\frac{1}{16} (231x^6 - 315x^4 + 105x^2 - 5)$
7	x^7	$\frac{1}{16} (429x^7 - 693x^5 + 315x^3 - 35x)$
8	x^8	$\frac{1}{128}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

Monomials: Degree of fit = 50

amplitudes

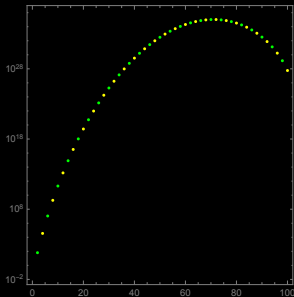


approximation

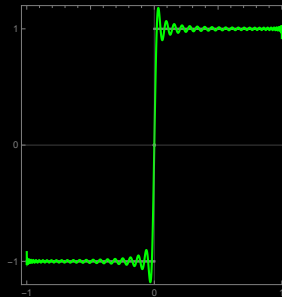


Monomials: Degree of fit = 100

amplitudes

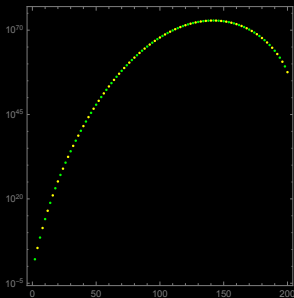


approximation

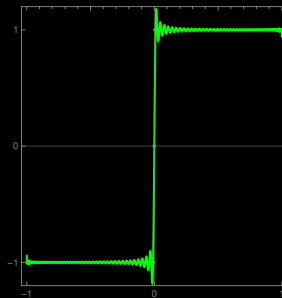


Monomials: Degree of fit = 200

amplitudes

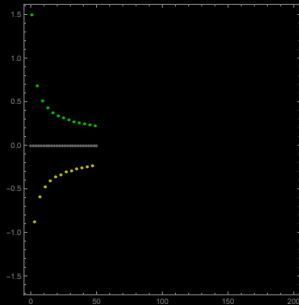


approximation

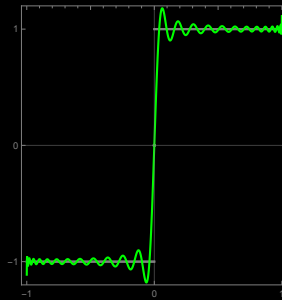


Legendre Polynomials: Degree of fit = 50

amplitudes

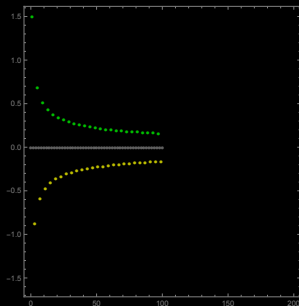


approximation

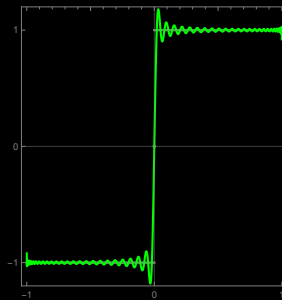


Legendre Polynomials: Degree of fit = 100

amplitudes

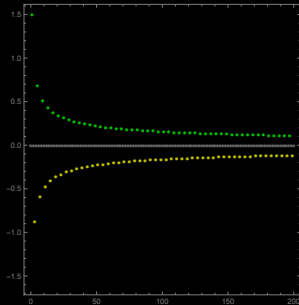


approximation

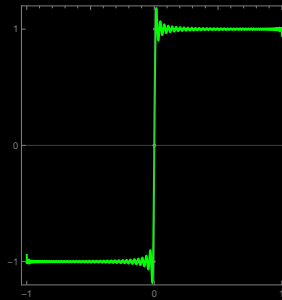


Legendre Polynomials: Degree of fit = 200

amplitudes



approximation



Computing in l^2

Lessons learned

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

Off-diagonal entries persist in l^2

Linearly independent system

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

Orthogonal system

$$\begin{bmatrix} \langle g_0|g_0 \rangle & 0 & \cdots & 0 \\ 0 & \langle g_1|g_1 \rangle & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \langle g_d|g_d \rangle \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_d \end{bmatrix} = \begin{bmatrix} \langle f|g_0 \rangle \\ \langle f|g_1 \rangle \\ \vdots \\ \langle f|g_d \rangle \end{bmatrix} \quad \perp$$

Quick Validation

Quick validation uncovers the loss of orthogonality.

Validation Tools

- 1 Simple construction
- 2 Simple interpretation
- 3 Display differences

Simple Example

Define

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

Compute

$$f(x) \approx b_0P_0(x) + b_1P_1(x) + b_2P_2(x) + b_3P_3(x) + b_4P_4(x) + \dots$$

Expectation

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

Solution vector

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

$$b = \{0, 1, 2, 3, 0, 0, 0\}$$

Function and Mesh

solve for amplitudes

input function

```
In[237]:= f[x_] = LegendreP[1, x] + 2 LegendreP[2, x] + 3 LegendreP[3, x];
```

$$f(x) = P_1(x) + 2P_2(x) + 3P_3(x)$$

mesh

```
In[232]:= Δ = 1/4;
```

```
mesh = Range[-1, 1, Δ]
```

```
Out[233]:= {-1, -3/4, -1/2, -1/4, 0, 1/4, 1/2, 3/4, 1}
```

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

linear system

$$\mathbf{A} = \begin{bmatrix} \int P_0(x)P_0(x)dx & \cdots & \int P_0(x)P_d(x)dx \\ \vdots & \ddots & \vdots \\ \int P_d(x)P_0(x)dx & \cdots & \int P_d(x)P_d(x)dx \end{bmatrix}$$

```
In[52]:= d = 6; (* order of fit *)
```

```
In[53]:= A = Table[
    LegendreP[row, mesh].LegendreP[col, mesh]
    , {row, 0, d}, {col, 0, d}];
```

$$\mathbf{y} = \begin{bmatrix} \int f(x)P_0(x)dx \\ \vdots \\ \int f(x)P_d(x)dx \end{bmatrix}$$

```
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}
```

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

Misapplication of L^2 Rules

faux-thonogonality

```
In[47]:= bfaux = Table[
    {k,  $\frac{2k+1}{2}$  f[mesh].LegendreP[k, mesh] Δ}
    , {k, 0, 6}];
% // N

Out[48]= {{0., 0.28125}, {1., 2.85645}, {2., 3.55957},
    {3., 8.00125}, {4., 3.41084}, {5., 9.47403}, {6., 6.05371}}
```

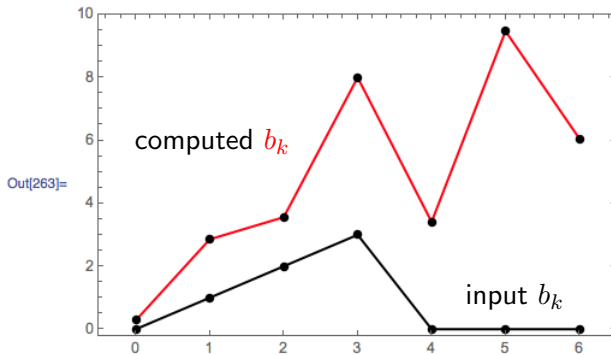
Misapplication of L^2 Rules

faux-thonogonality

```
In[47]:= bfaux = Table[
    {k,  $\frac{2k+1}{2} \int_{-1}^1 f(x) P_k(x) dx$  f[mesh].LegendreP[k, mesh] Δ}, b_k =  $\frac{\int_{-1}^1 f(x) P_k(x) dx}{\int_{-1}^1 P_k^* P_k(x) dx}$ 
    , {k, 0, 6}];
% // N

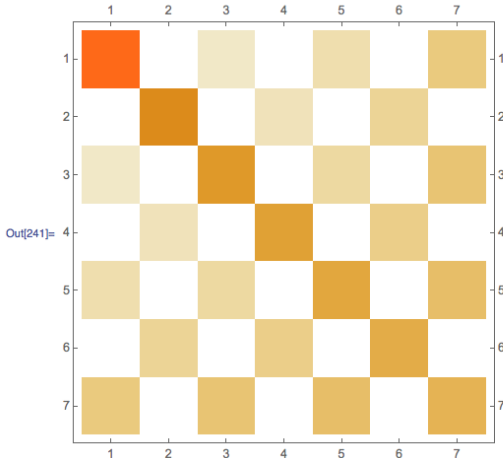
Out[48]= {{0., 0.28125}, {1., 2.85645}, {2., 3.55957},
    {3., 8.00125}, {4., 3.41084}, {5., 9.47403}, {6., 6.05371}}
```

Misapplication of L^2 Rules



Telling the Story with One Plot

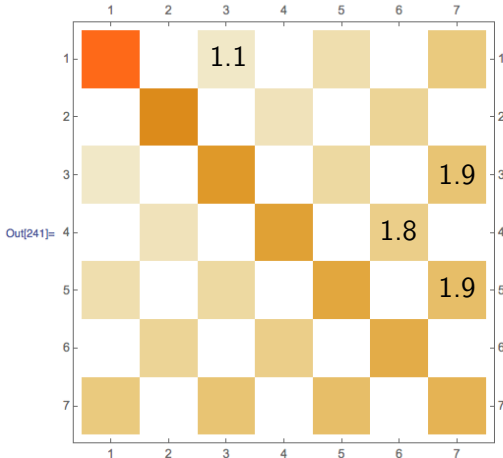
In[241]:= **MatrixPlot[Abs[A]]**



Not diagonal

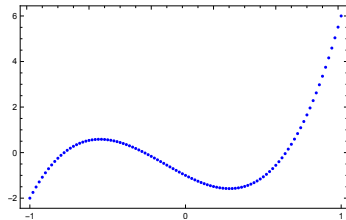
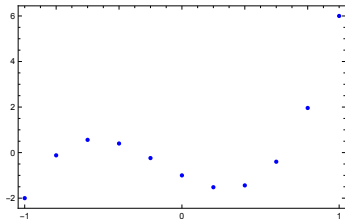
Telling the Story with One Plot

In[241]:= **MatrixPlot[Abs[A]]**

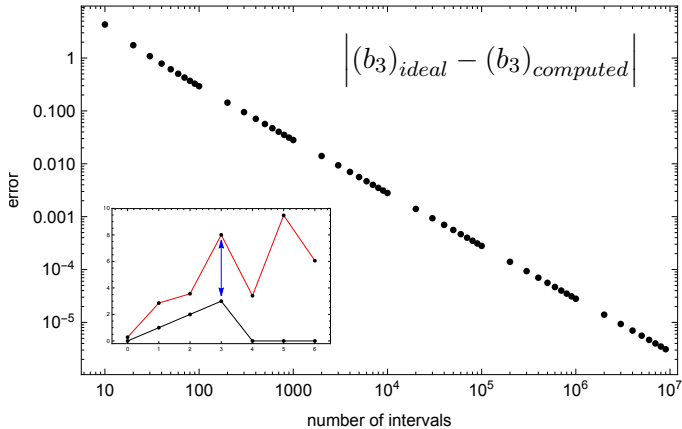


Not diagonal

Convergence: shrink interval



Convergence



Spreadsheet validation

Legendre amplitudes.xlsx

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SUMPRODUCT (H57:H515, D57:D515) * step * 5 / 2

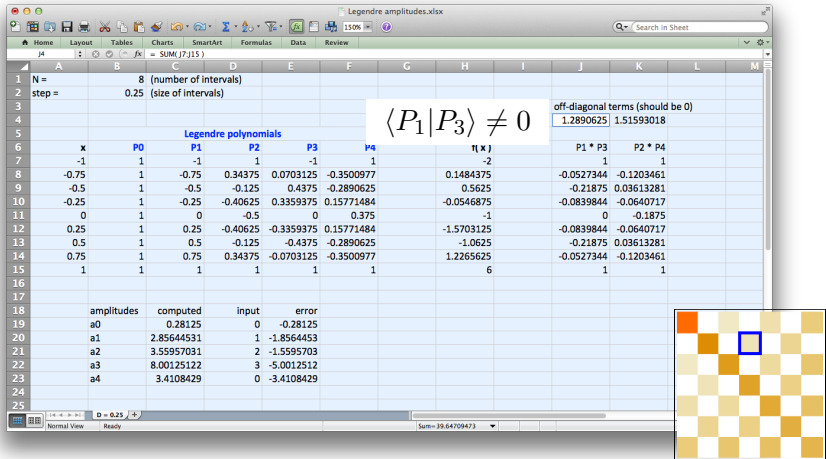
	A	B	C	D	E	F	G	H	I	J	K	L	M
1	N =	8	(number of intervals)										
2	step =	0.25	(size of intervals)										
3										off-diagonal terms (should be 0)			
4										1.2890625	1.51593018		
5			Legendre polynomials										
6	x	P0	P1	P2	P3	P4		f(x)		P1 * P3	P2 * P4		
7	-1	1	-1	1	-1	1		-2		1	1		
8	-0.75	1	-0.75	0.34375	0.0703125	-0.3500977		0.1484375		-0.0527344	-0.1203461		
9	-0.5	1	-0.5	-0.125	0.4375	-0.2890625		0.5625		-0.21875	0.03613281		
10	-0.25	1	-0.25	-0.40625	0.3359375	0.15771484		-0.0546875		-0.0839844	-0.0640717		
11	0	1	0	-0.5	0	0.375		-1		0	-0.1875		
12	0.25	1	0.25	-0.40625	-0.3359375	0.15771484		-1.5703125		-0.0839844	-0.0640717		
13	0.5	1	0.5	-0.125	-0.4375	-0.2890625		-1.0625		-0.21875	0.03613281		
14	0.75	1	0.75	0.34375	-0.0703125	-0.3500977		1.2265625		-0.0527344	-0.1203461		
15	1	1	1	1	1	1		6		1	1		
16													
17													
18		amplitudes	computed	input	error								
19		a0	0.28125	0	-0.28125								
20		a1	2.85644531	1	-1.8564453								
21		a2	= SUMPRODUCT(H57:H515, D57:D515) * step * 5 / 2										
22		a3	8.00125122	3	-5.0012512								
23		a4	3.4108429	0	-3.4108429								
24													
25													

D = 0.25

Normal View Edit

Sum=3.559570313

Spreadsheet validation



Spreadsheet validation

Legendre amplitudes.xlsx

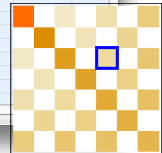
Home Layout Tables Charts SmartArt Formulas Data Review

K4 fx =SUM(K7:K15)

	A	B	C	D	E	F	G	H	I	J	K	L	M
1	N =	8	(number of intervals)										
2	step =	0.25	(size of intervals)										
3													
4										off-diagonal terms (should be			
5										1.2890625	1.51593018		
6			Legendre polynomials										
7	x	P0	P1	P2	P3	P4	f(x)	P1 * P3	P2 * P4				
8	-1	1	-1	1	-1	1	-2	1	1				
9	-0.75	1	-0.75	0.34375	0.0703125	-0.3500977	0.1484375	-0.0527344	-0.1203461				
10	-0.5	1	-0.5	-0.125	0.4375	-0.2890625	0.5625	-0.21875	0.03613281				
11	-0.25	1	-0.25	-0.40625	0.3359375	0.15771484	-0.0546875	-0.0839844	-0.0640717				
12	0	1	0	-0.5	0	0.375	-1	0	-0.1875				
13	0.25	1	0.25	-0.40625	-0.3359375	0.15771484	-1.5703125	-0.0839844	-0.0640717				
14	0.5	1	0.5	-0.125	-0.4375	-0.2890625	-1.0625	-0.21875	0.03613281				
15	0.75	1	0.75	0.34375	-0.0703125	-0.3500977	1.2265625	-0.0527344	-0.1203461				
16	1	1	1	1	1	1	6	1	1				
17													
18		amplitudes	computed	input	error								
19		a0	0.28125	0	-0.28125								
20		a1	2.85644531	1	-1.8564453								
21		a2	3.55957031	2	-1.5595703								
22		a3	8.00125122	3	-5.0012512								
23		a4	3.4108429	0	-3.4108429								
24													
25													

Normal View Ready D = 0.25 Sum=39.64709473

$$\langle P_2 | P_4 \rangle \neq 0$$



Validation Results

- Simple tools uncover problem
- Better tools point to solution

Orthogonality and Computation

Daniel Topa

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ERDC DSRC
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Monday 25th January, 2016