Orthogonality and Computation

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Overview

CAUTION

when using orthogonal functions in discrete spaces

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

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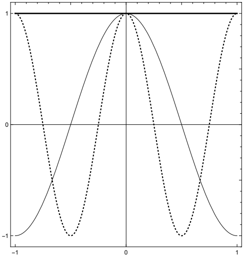

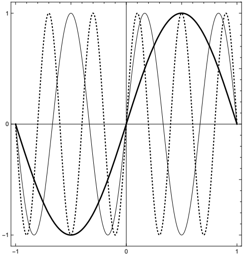

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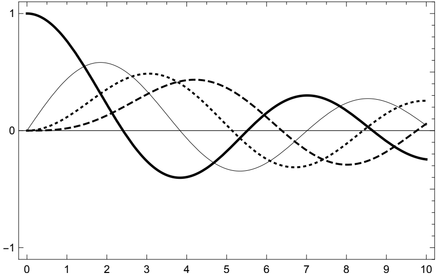

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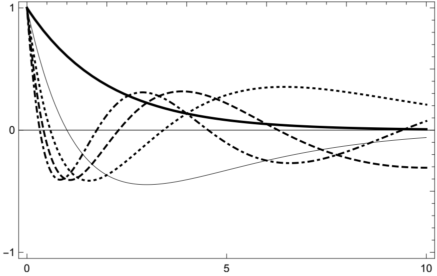

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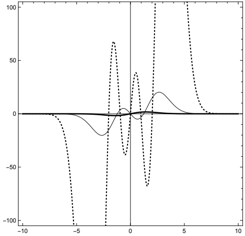

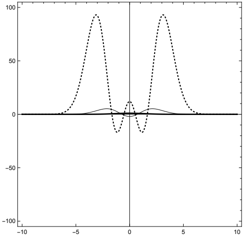

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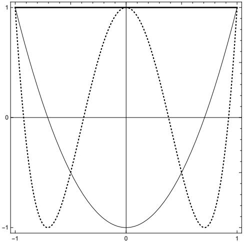

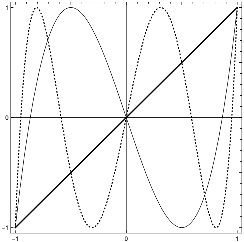

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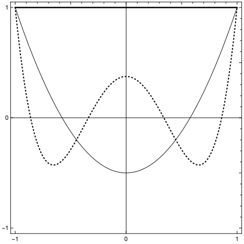

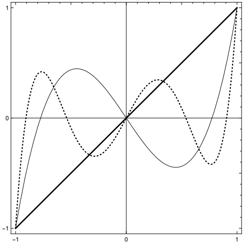

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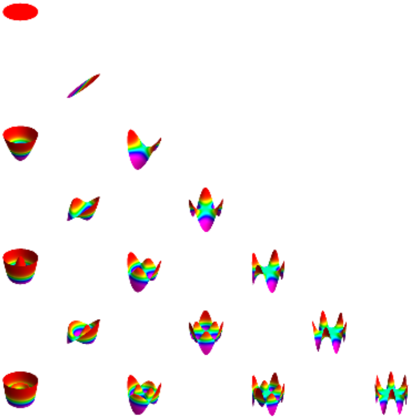

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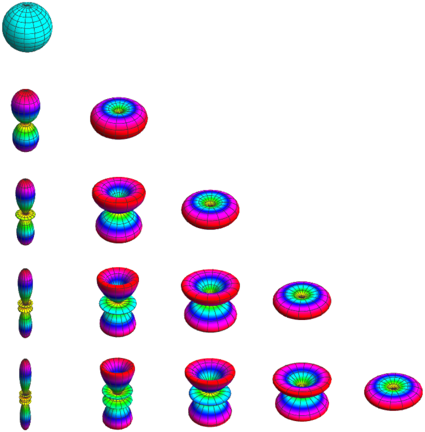

Orthogonal functions

Popular functions orthogonal in computation

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Critical observation

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

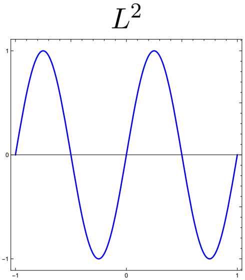
$$\sin nx, \quad \cos nx$$

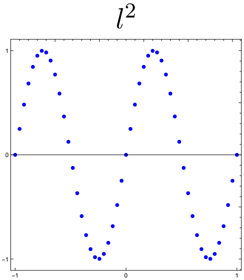
Rudiments

Orthogonality depends upon

1. domain
2. topology (continuous or discrete)

Snapshot





L^2 is not l^2

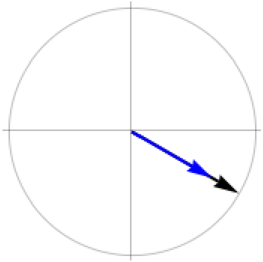
That's why they have different symbols

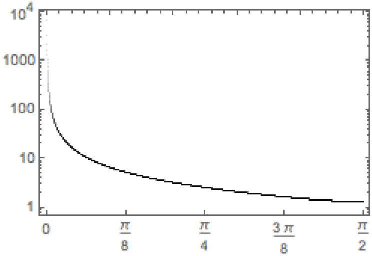
Prototype linear equation

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

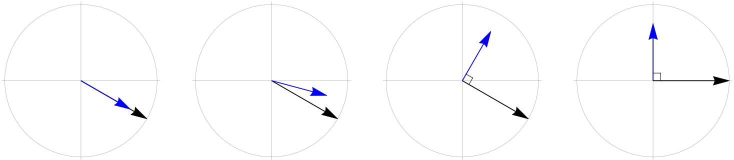
$$x_1 \begin{bmatrix} a_{11} \\ \vdots \\ a_{m1} \end{bmatrix} + \cdots + x_n \begin{bmatrix} a_{1n} \\ \vdots \\ a_{mn} \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix}$$

Condition Number



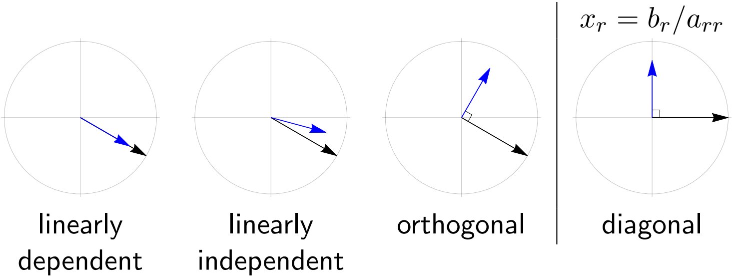


Column vectors of $\mathbf{A}$

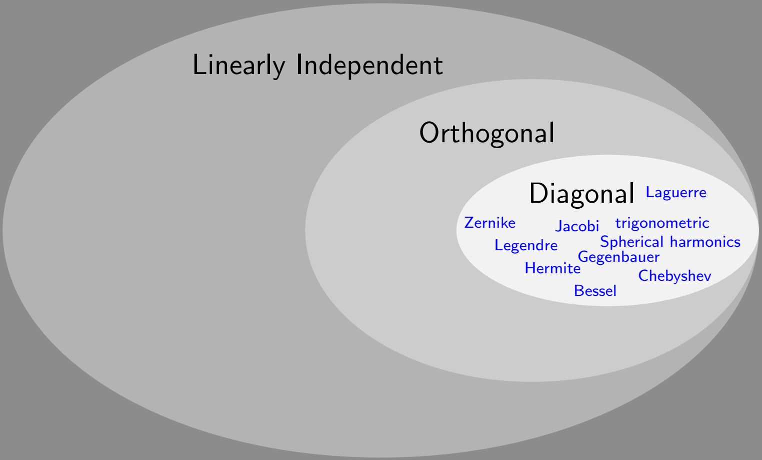


linearly dependent | linearly independent | orthogonal | diagonal

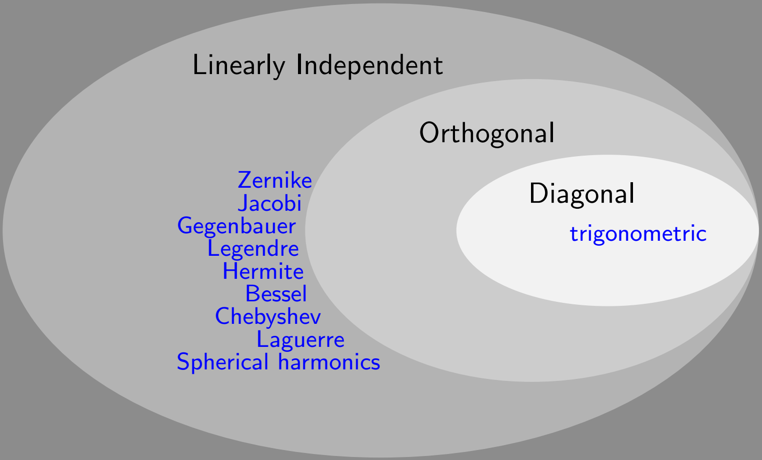
Column vectors of $\mathbf{A}$: clicks



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

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

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

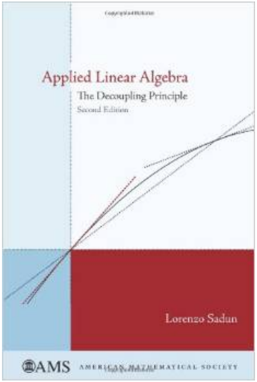
$$\Downarrow$$

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

Decoupling Principle

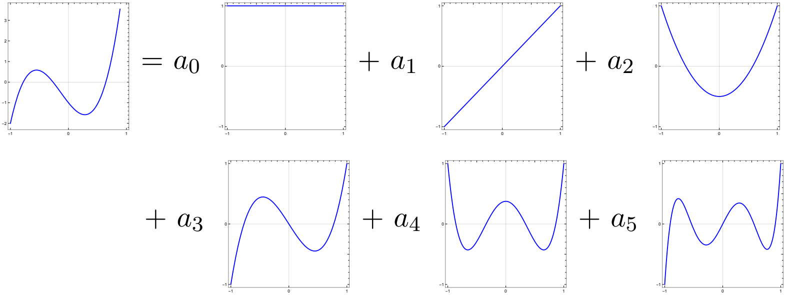
Diagonal Systems are Decoupled

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



L^2: Legendre Basis

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



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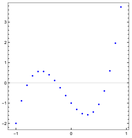
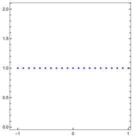
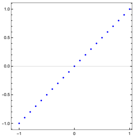
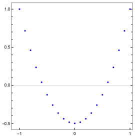
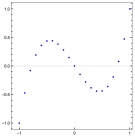
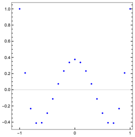
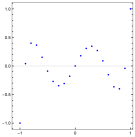
 $=\; b_0$  $+\; b_1$  $+\; b_2$ 

$+\; b_3$  $+\; b_4$  $+\; b_5$ 

Finding the Amplitudes

Finding amplitudes = Solving linear systems

Formalities

Orthogonality and Computation

CSC'15

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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

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

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.

Riesz-Fischer

Theorem 1 (Riesz–Fischer)

Let $\{\phi_n\}$ be an orthonormal sequence of functions on Ω and suppose $\sum |a_n|^2$ converges. Denote the partial sum as

$$s_d = a_0\phi_0 + a_1\phi_1 + \cdots + a_d\phi_d.$$

There exists a function $F \in L^2(\Omega)$ such that $\{s_d\}$ converges to F in $L^2(\Omega)$, and such that

$$F = \sum_{k=0}^{\infty} a_k\phi_k,$$

almost everywhere.

Normal Equations: General Case

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

Expression of Orthogonality

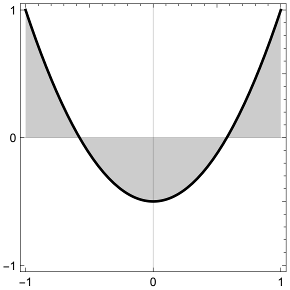
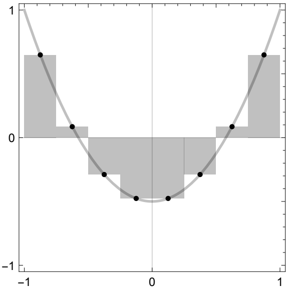
$$m \neq n$$

$$
\begin{array}{lcccc}
L^2\colon & \langle G_m | G_n \rangle & = & \int\limits_{\Omega} G_m(x) G_n(x) dx & = & 0 \\
l^2\colon & \langle g_m | g_n \rangle & = & \sum\limits_{x \in \sigma} g_m(x) g_n(x) \Delta & = & 0
\end{array}
$$

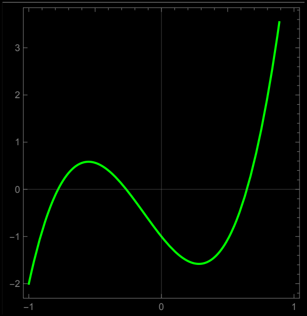
Normal Equations: Orthogonal Basis

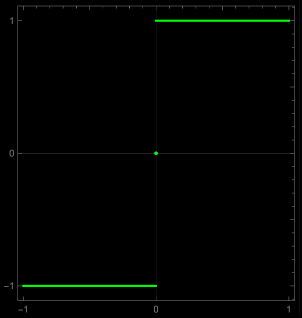
$$
\begin{array}{cccc}
 & \text{system} & \text{sol'n} & & \text{data} \\
L^2: & \begin{bmatrix} \langle G_0|G_0\rangle & 0 & \cdots & 0 \\ 0 & \langle G_1|G_1\rangle & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \langle G_d|G_d\rangle \end{bmatrix} & \begin{bmatrix} a_0 \\ a_1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

In a Nutshell

L^2	l^2
	
$\langle G_m \vert G_n \rangle$	$\langle g_m \vert g_n \rangle$
$\int_\Omega P_m(x) P_n(x) dx = 0$	$\sum_{x \in \sigma} P_m(x) P_n(x) \Delta \neq 0$

Smoothness





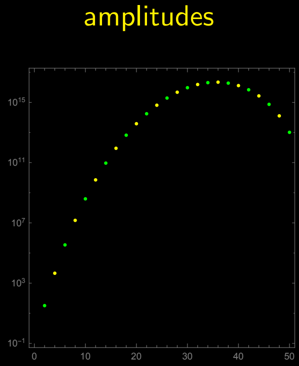
Monomials and Legendre Polynomials

k	$M_k(x)$	$P_k(x)$
0	1	1
1	x	x
2	x^2	$\frac{1}{2}\left(3x^2-1\right)$
3	x^3	$\frac{1}{2}\left(5x^3-3x\right)$
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	$\frac{1}{128}\left(12155x^9-25740x^7+18018x^5-4620x^3+315x\right)$
10	x^{10}	$\frac{1}{256}\left(46189x^{10}-109395x^8+90090x^6-30030x^4+3465x^2-63\right)$

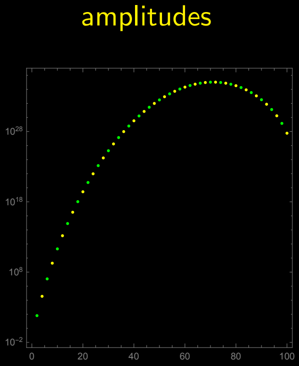
Comparing methods

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

Monomials: Degree of fit = 50

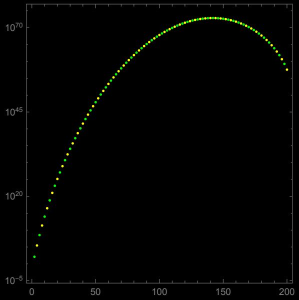


Monomials: Degree of fit = 100

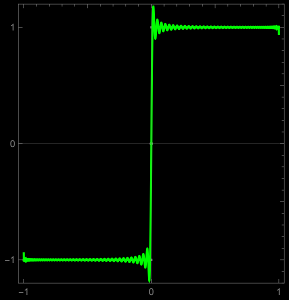


Monomials: Degree of fit = 200

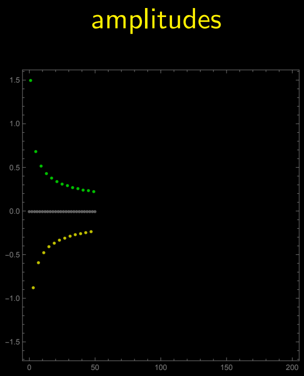
amplitudes



approximation

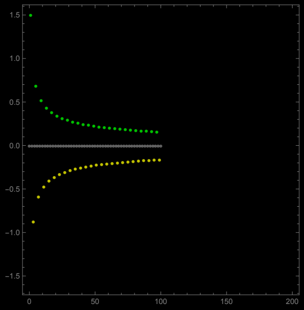


Legendre Polynomials: Degree of fit = 50



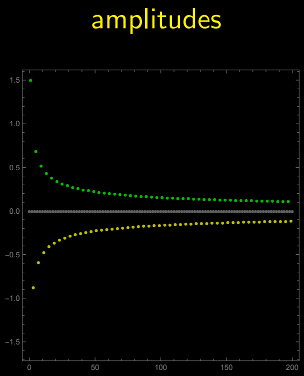
Legendre Polynomials: Degree of fit = 100

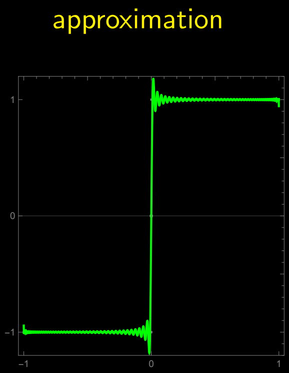
amplitudes



approximation

Legendre Polynomials: Degree of fit = 200





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

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

Orthogonal system

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

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

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

Expectation

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

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

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

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}];
```

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

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

solution

```
In[55]:= btrue = Inverse[A].y

Out[55]= {0, 1, 2, 3, 0, 0, 0}
```

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

Misapplication of L^2 Rules

faux-thogonality

```
In[47]:= bfaux = Table[
           {k, (2 k + 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-thogonality

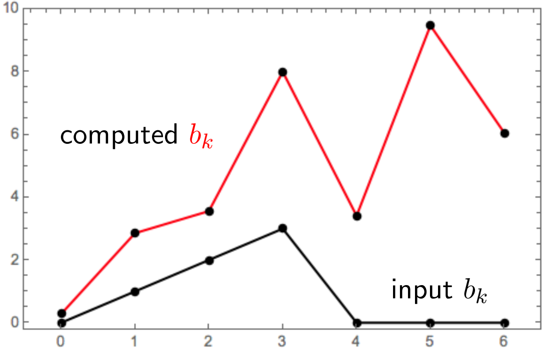
```
In[47]:= bfaux = Table[
           {k, (2 k + 1)/2 f[mesh].LegendreP[k, mesh] Δ}
           , {k, 0, 6}];
         % // N

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

$$b_k = \frac{\int_{-1}^{1} f(x) P_k(x) dx}{\int_{-1}^{1} P_k^* P_k(x) dx}$$

Misapplication of L^2 Rules

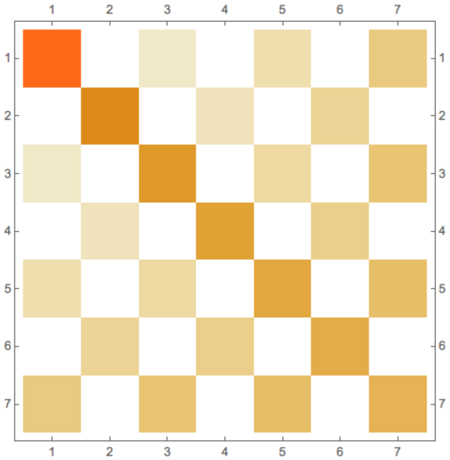
Out[263]=



Telling the Story with One Plot

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

Out[241]=

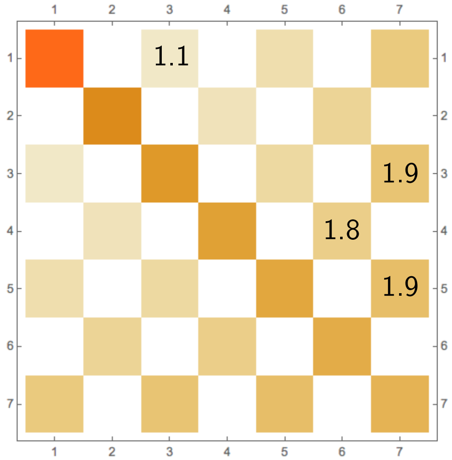


Not diagonal

Telling the Story with One Plot

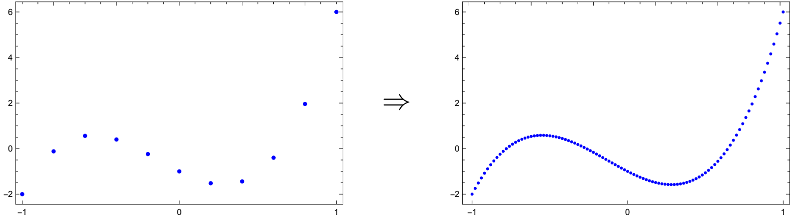
In[241]:= `MatrixPlot[Abs[A]]`

Out[241]=

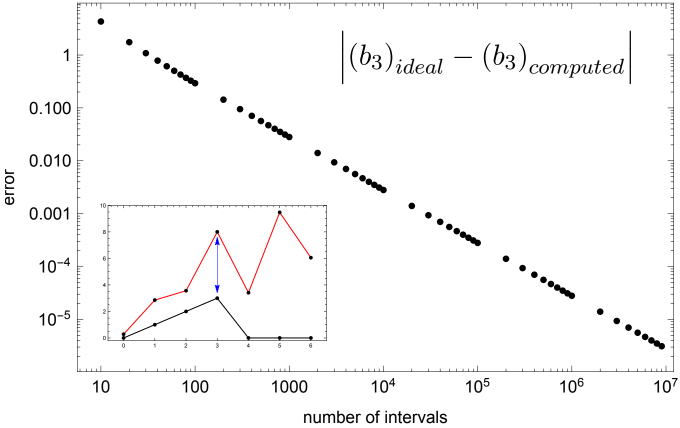


Not diagonal

Convergence: shrink partition



Convergence



Spreadsheet validation

Legendre amplitudes.xlsx

Home | Layout | Tables | Charts | SmartArt | Formulas | Data | Review

SUMPRODUCT = SUMPRODUCT(H$7:H$15, D$7:D$15) * step * 5 / 2

	A	B	C	D	E	F	H	J	K
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(H$7:H$15, D$7:D$15) * 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

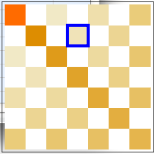
Legendre amplitudes.xlsx

J4 = SUM(J7:J15)

	A	B	C	D	E	F	G	H	I	J	K
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	3.55957031	2	-1.5595703						
22		a3	8.00125122	3	-5.0012512						
23		a4	3.4108429	0	-3.4108429						
24											
25											

D = 0.25 — Normal View — Ready — Sum= 39.64709473

$$\langle P_1 | P_3 \rangle \neq 0$$



Spreadsheet validation

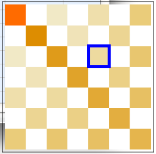
Legendre amplitudes.xlsx

K4 f_x = SUM(K7:K15)

	A	B	C	D	E	F	G	H	I	J	K
1	N =	8	(number of intervals)								
2	step =	0.25	(size of intervals)								
3										off-diagonal terms (should be	
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	3.55957031	2	-1.5595703						
22		a3	8.00125122	3	-5.0012512						
23		a4	3.4108429	0	-3.4108429						
24											
25											

D = 0.25 — Normal View — Ready — 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

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Tuesday 7th June, 2016