Vectors

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Orthonormal bases of functions

April 24, 2018

Data - Vectors or Functions	Vectors	Functions	Popular functional bases
Outline			



Data - Vectors or Functions







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Functions

Popular functional bases

Downloading R-package and first steps

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Downloading R-package and first steps

Statistical R-package available for free download here

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- Statistical R-package available for free download here
- Available on any PC platform (Mac, Windows, Linux).

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- Worry free and fast downloading procedure (a couple of minutes).

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- We will be working in the command line window of R (most direct way of accessing R-package).
- No experience is required all of the code that will be needed will be provided on our webpage!
- There some so-called R front-ends (such R Commander or R-Studio or Jupyter) that ease writing more complex programming in R – while you can use and utilize them, I assume **only a very basic R installation** with the primitive *copy-and-paste-to-the-command-line* approach as a method of running the programs.

Getting access to 'fda' package

- After installing R, any package available on the r-project webpage can be easily downloaded and installed on individual computers.
- This also applies to 'fda' package.
- The instructions for downloading and launching a package differ depending on platform.
- All are however straightforward and take no longer than a minute.
- In the package are all scripts that have been used in our main textbook.

system.file('scripts	', package='fda	')			
# [1] "/Users/mats-k	sp/Library/R/3.	4/library/fda/s	cripts"		
dir("/Users/mats-ks	p/Library/R/3.4	/library/fda/sc:	ripts")		
# [1] "afda-ch01.R"	"afda-ch02.R"	"afda-ch03.R"	"afda-ch04.R"	"afda-ch05.R"	"afda-
# [7] "afda-ch07.R"	"fda-ch01.R"	"fda-ch02.R"	"fda-ch03.R"	"fda-ch07.R"	"fda-c
#[13] "fda-ch13.R"	"fda-ch17.R"	"fdarm-ch01.R"	"fdarm-ch02.R"	"fdarm-ch03.R"	"fdarm
#[19] "fdarm-ch05.R"	"fdarm-ch06.R"	"fdarm-ch07.R"	"fdarm-ch08.R"	"fdarm-ch09.R"	"fdarm
#[25] "fdarm-ch11.R"					
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Vectors

Functions

Popular functional bases

Example of a very simple R session with fda package

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Data - Vectors or Functions	Vectors	Functions	Popular functional bases
Example of a very simp	le R session wit	th fda package	
This is based of package.	n the script "afda	a-ch01.R " availabe	in the fda

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Example of a very simple R session with fda package

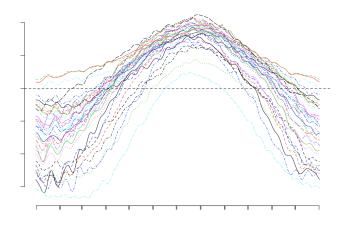
- This is based on the script "afda-ch01.R" availabe in the fda package.
- If the following lines of code do not create the error messages then the package is properly installed:

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Smoothed Canadian weather



• Few lines of the code from the previous result should produce



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Canadian average annual weather cycle

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Canadian average annual weather cycle

- Description: Daily temperature and precipitation at 35 different locations in Canada averaged over 1960 to 1994.
- CanadianWeather is a list with the following components:
 - dailyAv: a three dimensional array c(365, 35, 3) summarizing data collected at 35 different weather stations in Canada on the following:
 - [,,1] = [,, 'Temperature.C']: average daily temperature for each day of the year
 - [,,2] = [,, 'Precipitation.mm']: average daily rainfall for each day of the year rounded to 0.1 mm.
 - [.,3] = [., 'log10precip']: base 10 logarithm of Precipitation.mm after first replacing 27 zeros by 0.05 mm.
 - place: Names of the 35 different weather stations in Canada whose data are summarized in 'dailyAv'. These names vary between 6 and 11 characters in length. By contrast, daily[["place"]] which are all 11 characters, with names having fewer characters being extended with trailing blanks.
 - province: names of the Canadian province containing each place
 - coordinates: a numeric matrix giving 'N.latitude' and 'W.longitude' for each place.
 - region: Which of 4 climate zones contain each place: Atlantic, Pacific, Continental, Arctic.
 - monthlyTemp: A matrix of dimensions (12, 35) giving the average temperature in degrees celcius for each month of the year.
 - monthlyPrecip: A matrix of dimensions (12, 35) giving the average daily precipitation in milimeters for each month of the year.
 - geogindex: Order the weather stations from East to West to North

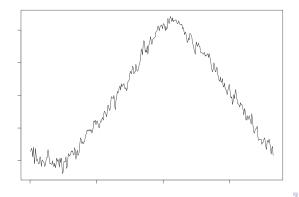
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A sample from one station

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- Extracting temperature and plotting it for the first station a=CanadianWeather\$dailyAv[,, "Temperature.C"] plot(a[,1],type="l")
- The result



- We have seen an example of data for which a functional data analysis will be applied.
- If one considers a single location, a sample is a 365 dimensional vector of averaged daily temperatures.
- The vector of this size can be easily analyzed using multivariate analysis.

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• Why do we want to use functions?

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Outline			





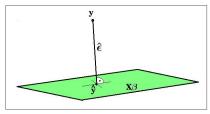








• A picture to have in mind



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- Inner product.
- Orthogonality.
- Dimension.
- Orthogonal projections

Data - Vectors or Functions	Vectors	Functions	Popular functional bases
Inner product			

- Defintion.
- Properties.
- Geometric interpretation.

Data - Vectors or Functions	Vectors	Functions	Popular functional bases
Orthogonality			

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- Definition.
- Pythagorean Theorem.
- Geometric interpretation.

Data - Vectors or Functions	Vectors	Functions	Popular functional bases
Dimension			

- Definition of a linear basis.
- Orthogonal bases.
- Dimension.

Data - Vectors or Functions	Vectors	Functions	Popular functional bases
Linear operations - mati	rices		

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- Linear transformation (linear operator).
- Representation as a matrix.

Linear regression – example of vector valued conceptualization

- We have response variables Y = (Y₁,..., Y_n) and a matrix of regressor (explanatory variables) X = [x_{ij}]^{n,r}_{i=1}.
- The assumed model is

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}.$$

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- Here β is an unknown vector of the parameters and ϵ is a random noise.
- The goal is to estimate β given the set of observations (Y, X).



 In the least square approach, one estimates β by minimizing the Eucledean distance between the observations and the linear model

 $\|\mathbf{y}-\mathbf{X}\boldsymbol{\beta}\|^2.$

- In other words, we want to find a point β̂ such that Xβ̂ is the closet point to the observations y among all Xβ's.
- It follows from the principles of linear algebra that Xβ is the orthogonal projection ŷ of the observation vector y to the space of spanned by the columns of the design matrix X. This projection can be expressed as the matrix P = X(X'X)⁻¹X', so that

$$\hat{\mathbf{y}} = \mathbf{P}\mathbf{y}$$

 $\hat{oldsymbol{eta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$

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Because:

- The vector based analysis is invariant on the permutations of coordinates of vectors. Think about the analysis of the Canadian weather data after randomly permuting coordinates.
- The dimension reduction: high dimensional data maybe represented using few functions (one function has infinitely many coordinates so the size does not matter).
- Certain problems can be only expressed in the functional terms: increase of the sampling frequency of the data, search for an efficient way of representing certain structural features in the data – selection of the basis and its optimality (think images).
- Possibility of using operations that are specific for functions: derivatives, integrals.
- Certain physical phenomena are conveniently described through functions and their derivatives: response to a signal.

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Finally,

Because:

- The vector based analysis is invariant on the permutations of coordinates of vectors. Think about the analysis of the Canadian weather data after randomly permuting coordinates.
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Finally, why not? The theory is not that much different.

- Hilbert space: A collection of vectors with all properties the same as in Euclidean space except finite dimensionality.
 - Functions constitute a Hilbert space (there are also other Hilbert spaces).
 - A Hilbert space with a countable a basis {*e_k*, *k* ∈ *Z*}) with inner product ⟨·, ·⟩ which generates norm || · ||

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Samples in functional spaces

- An important example is the Hilbert space $L^2 = L^2([0, 1])$, which is the set of measurable real-valued functions x defined on [0,1] satisfying $\int_0^1 x(t)^2 dt < \infty$.
- Observations are random functions i.e. random variables defined on some common probability space (Ω, A, P) with values in L^2 .
- We say that X is integrable if $E||X|| < \infty$ and square integrable if $E\|X\|^2 < \infty.$

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- There are several versions of Fourier bases but they all express in terms of sines and cosines.
- The most standard is

$$\{\sqrt{2}\sin(2\pi nx); n \in \mathbb{N}\} \cup \{\sqrt{2}\cos(2\pi nx); n \in \mathbb{N}\} \cup \{1\}.$$

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Two alternatives are the sine basis

$$\{\sqrt{2}\sin(\pi nx); n \in \mathbb{N}\}$$

and the cosine basis

$$\{\sqrt{2}\cos(\pi nx); n \in \mathbb{N}\} \cup \{1\}.$$

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Fourier bases in R - a direct approach

```
#Fourier basis
nb=45
```

```
n=2002 #size of the equidistant one dimensional grid
h=1/n #increment size
t=matrix(seq(h,1,by=h),ncol=1) #grid
```

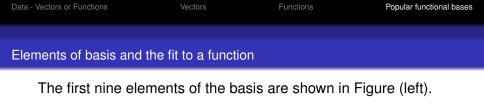
```
Fbase=matrix(0,ncol=n,nrow=nb) #matrix of basis values
```

```
Sn=matrix (2*(1:floor (nb/2)), ncol=1)
Cn=matrix (2*(1:ceiling (nb/2))-1, ncol=1)
```

```
Fbase[Sn,]=sqrt(2)*sin(pi*Sn% (t)) #sin in basis
Fbase[Cn,]=sqrt(2)*cos(pi*(Cn-1)% (t)) #cos in basis
Fbase[1,]=Fbase[1,]/sqrt(2)
```

```
plot(t,Fbase[2,],type="1", col=2,ylab="")
lines(t,Fbase[1,],type="1", col="red")
for(i in 3:9)
{
lines(t,Fbase[i,],type="1", col=i)
}
```

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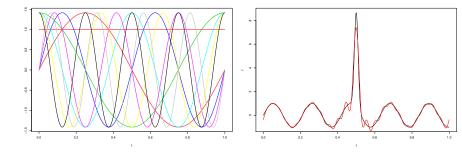


Figure: Fourier basis – *(left)*. A function (in black) and its approximation by an expansion in the Fourier basis (in red) – *(right)*.

The code and the theory – least squares

- One important benefit of using these basis is availability of effective computational algorithm, the Fast Fourier Transform (FFT), for evaluation of the basis expansion coefficients.
- However, in our considerations, we will not benefit greatly from this algorithm so we rather compute the coefficient in a more direct way as shown in the next code.

```
#Test function and its plot
f=t(8*exp(-5000*(t-1/2)^2)+sin(30*t))
plot(t,f,type="1")
#Computation of coefficients
```

Cf=f%*%t(Fbase)*h

#Computation of expansion (projections) Pf=Cf%*%Fbase

```
#Plot of the projection
lines(t,Pf,type="l",col='red')
```

We can see from the code that it is just the regular least square method applied to the functions.

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More on the least squares in the expansion of a function

- O-U basis
- Coefficients of expansion.
- Pythagorean theorem and the optimality of the reminder.

- It follows from the Stone-Weirstrass theorem that every continuous function defined on [0, 1] can be uniformly approximated as closely as desired by a polynomial function.
- Thus at the first sight, it seems reasonable to consider polynomial bases.
- An obvious normalized while not orthonormal basis is the following sequence of monomials

$$\{\sqrt{2n+1} x^n; n \in \mathbb{N}_0\},\tag{1}$$

where $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$.

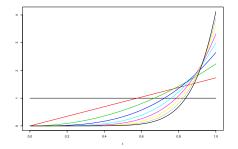
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The elements of this basis are shown in Figure and computed using the following code.

```
#Plotting monomial basis
nb=45
n=2002
h=1/n
t=matrix(seg(h,1,by=h),ncol=1) #grid
n=dim(t)[1]
i = 0
Mono=matrix (1, ncol=nb, nrow=n)
Mono[.1] = sort(2*i+1)*matrix(1.ncol=1.nrow=n)
for(i in 1:(nb-1))
 Mono[, i +1]=(((2*i+1)^(1/(2*i)))*t)^i
Max=max(Mono[,1:15])
Min=min (Mono[,1:15])
plot(t,Mono[,1],type='l',ylim=c(Min,Max),ylab='')
for(i in 2:15)
  lines(t,Mono[,i],type='l',col=i)
}
```

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Graphs			



- The monomial basis
- How to make these polynomials orthogonal (orthonormal)?

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 For a sequence of linearly independent elements *h_n* ∈ *H*, *n* ∈ N₀, *H* is some Hilbert space, the Gram-Schmidt orthonormalization of *h_n* defines an orthonormalized vectors *e_n*, *n* ∈ N₀, through the following recurrence

$$e_0 = h_0 / \|h_0\|$$

$$e_{n+1} = \alpha_n e_n + \beta_{n+1} h_{n+1}, n \in \mathbb{N}_0,$$

where

$$\alpha_n = -\beta_{n+1} \langle e_n, h_{n+1} \rangle, \quad \beta_{n+1}^2 = \frac{1}{\|h_{n+1}\|^2 - |\langle e_n, h_{n+1} \rangle|^2}.$$

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Orthonormalization of polynomials

- It is clear that the sequence of the polynomials obtained through this procedure has increasing order.
- The coefficients of these polynomials can be obtained algebraically through the following simple recurrent linear procedure.
- Let h_k, k = 1, ..., n, be represented as a sequence of numerical vectors a_k, k = 1, ..., n, in a certain basis (not necessarily orthonormal and its form is irrelevant for the procedure).
- Moreover let $\mathbf{H} = \left[\langle h_i, h_j \rangle \right]_{i,j=0}^n$.
- Define b₀ = a₀/||h₀|| = a₀/√h₀₀, which is the representation of the first vector of the G-S orthonormal basis.
- The second vector can be obtained by defining first

$$\tilde{\mathbf{a}}_k = \mathbf{a}_k - \frac{h_{k0}}{h_{00}} \mathbf{a}_0, \ k = 1, \dots, n$$
$$\tilde{\mathbf{H}} = \left[h_{ij} - \frac{h_{i0}h_{0j}}{h_{00}} \right]_{i,j=0}^n$$

and then taking $\mathbf{b}_1 = \tilde{\mathbf{a}}_1 / \sqrt{\tilde{h}_{11}}$.

Moreover, to find the next vector b₂, one applies the same procedure (but by one dimension smaller) to ã and H
in place of a and H.

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This approach is implemented in the following routine.

```
#Implementation of Gram-Schmidt orthonormalization
gso=function(A,H)
 nb=dim(H)[1]
  k=dim(A)[1]
 HH=H
 AA=A
  B=A #the k x nb. k \ge nb matrix output with columns being orthonormalized columns of A
  i =1
  B[,1]=AA[,1, drop=F]/HH[1,1] #the first output vector normalized
  while (nb>1){
    H1=HH[1..drop=F]
                                # row 1 x nb
    AA=AA-(H1%x%AA[,1, drop=F])/HH[1,1]
                                                #kxnb
    HH=HH-t (H1)%*%H1/HH[1,1]
    HH=HH[2:nb,2:nb, drop=F]
    AA=AA[,2:nb,drop=F]
    i = i + 1
    B[,i]=AA[,1,drop=F]/sqrt(HH[1,1]) #subsequent column to the output
    nb=nb-1
В
}
```

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Back to polynomials

We note that for the monomial basis the matrix of the inner products is given by

$$\mathbf{H} = \left[\frac{\sqrt{2i+1}\sqrt{2j+1}}{i+j+1}\right]$$

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```
Thus the following program computes the orthonormal basis.
```

```
#G-S orthonormalization
nb=12
A=diag(nb)
```

```
I = t(rep(1.nb))
S=0:(nb-1)
H=1/(I\%\%\%S+1/2+t(I\%\%\%S+1/2))
S=(sqrt(2*S+1))%*%t(sqrt(2*S+1))
H=H*S
```

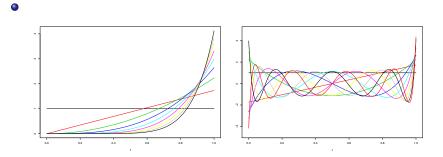
B=gso(A,H)

#Plotting orthonormal polynomial basis

```
PBase=matrix(1,ncol=nb,nrow=n)
PBase=Mono[,1:nb]%*%B
Max=max(PBase[,1:nb])
Min=min(PBase[,1:nb])
plot(t, PBase[,1], type='l', ylim=c(Min, Max), ylab='')
for(i in 2:10)
  lines(t, PBase[, i], type='|', col=i)
```

Data - Vectors or Functions	Vectors	Functions	Popular functional bases

Basis vs Orthornormal basis



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Instability and approximation

- The resulting orthonormal basis was illustrated in Figure.
- Unfortunately, the choice of initial monomials is not wise due to the numerical instability of the
 orthonormalization of so similarly looking functions.
- Due to this the routine crashes after 13 iterations.
- The routine for computing the expansion of a function is similar as before.

```
#The test function
plot(t,f,type="l")
```

#Computation of coefficients

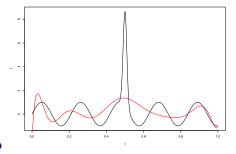
Cf=f%*%t(PBase)*h

```
#Computation of expansion (projections)
Pf=Cf%*%PBase
```

```
#Plot of the projection
lines(t,Pf,type="l",col='red')
```

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Data - Vectors or Functions	Vectors	Functions	Popular functional bases
Performance			



The approximation using 13 elements of the orthonormalized polynomial basis - *(left)*. We see that 13 polynomials perform poorly.

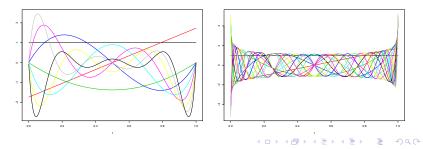
Data - Vectors or Functions	Vectors	Functions	Popular functional bases
Stabilizing			

To have more fair comparison with the Fourier expansion we need more elements of the orthonormal basis and for this one has to start with a better polynomial basis.

In fact, it will be more numerically stable to start with the following functions

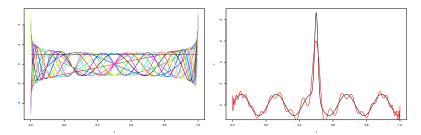
$$\begin{split} &h_0(x) = 1, \\ &h_1(x) = x - 1/2, \\ &h_n(x) = \frac{\sqrt{2}}{2e} \prod_{i=0}^{n-1} \left(2\sqrt{e n} \left(x - \frac{i}{n-1} \right) \right), \ n \geq 2, \end{split}$$

as their provide more variability as shown in the plot, where h_n are normalized before being drawn. A numerically stable initial polynomial basis – (*left*) and the orthonormalized output from the G-S procedure (*right*).



Performance with more basis functions

- The orthonormal polynomial is again attempted using the previous G-S routine and this time 45 elements is obtained and 16 of their elements are shown in Figure (*left*).
- We observe that the polynomial expansion still does not perform as well as the trigonometric expansion.



16 elements of the orthonormalized polynomial basis – *(left)*. An approximation of the test function with all 45 elements– *(right)*.

Data - Vectors or Functions	Vectors	Functions	Popular functional bases
Conclusions			

- An important lesson from the polynomial basis example is that a choice of the basis may greatly affect the performance of numerical algorithms, even if in the mathematical terms this should not create a problem.
- In fact we have seen that the unique polynomial basis on interval [0, 1] could not be effectively computed if the initial choice of the polynomials was not screened for the variability (the case of the monomials).
- The numerical problem disappeared by considering 'less linearly dependent' initial basis.
- From the mathematical point of view the two bases were equivalent but for computational purposes one performed poorly and the other was quite reasonable.
- Approximation using monomial polynomials is not numerically effective but through a more suitable initial choice of the linear basis to be orthogonalized we arrived to better numerical stability of the Gram-Schmidt orthonormalization.

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Data - Vectors or Functions	Vectors	Functions	Popular functional bases

Analytical solution to the problem of polynomial ON basis

- The good news is that for the case of the orthonormal basis of polynomials on an interval we have an analytical solution to the problem and thus the problem of stability discussed in the previous slides can be avoided.
- It can be derived analytically also using the Gram-Schmidt orthogonalization process to the basis 1, x, x²,
- It will be convenient to present the solution on interval [-1, 1] rather than on [0, 1] but the following transformation leads from the [-1, 1] case to the case of [0, 1]:

$$\tilde{f}(y) = \frac{\sqrt{2}}{2}f\left(\frac{y+1}{2}\right).$$

Data - Vectors	s or Functions	Vectors	Functions	Popular functional b	ases
Legendr	e polynomials				
۲	The elements of the resulting definition is given next.	basis for [—1, 1] are known	as the Legendre polynomial ar	nd their recurrent	
Definit	ion				

The Legendre polynomials, denoted by $L_k(x)$, are the orthogonal polynomials in $L^2(-1, 1)$. The three-term recurrence relation for the Legendre polynomials reads

$$\begin{split} L_0(x) &= 1, \\ L_1(x) &= x, \\ (n+1)L_{n+1}(x) &= (2n+1)xL_n(x) - nL_{n-1}(x), n \geq 1. \end{split}$$

Theorem

For $n, m \ge 0$ and $x \in [-1, 1]$ we have

$$\int_{-1}^{1} L_m(x) L_n(x) \, dx = \frac{2}{2n+1} \, \delta_{mn},$$

and an explicit form of the Legendre polynomials as

$$L_{n}(x) = \sum_{k=0}^{n} (-1)^{k} {\binom{n}{k}}^{2} \left(\frac{1+x}{2}\right)^{n-k} \left(\frac{1-x}{2}\right)^{k}$$

• The theorem above shows that the Legendre polynomials are orthogonal in $L^2(-1, 1)$.

The first six Legendre polynomials are:

$$L_{0}(x) = 1,$$

$$L_{1}(x) = x,$$

$$L_{2}(x) = \frac{1}{2}(3x^{2} - 1),$$

$$L_{3}(x) = \frac{1}{2}(5x^{3} - 3x),$$

$$L_{4}(x) = \frac{1}{8}(35x^{4} - 30x^{2} + 3),$$

$$L_{5}(x) = \frac{1}{8}(63x^{5} - 70x^{3} + 15x)$$

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- While restricting to an interval and considering functions only on an interval is often practically valid, it may happen that restricting to a specific interval will appear artificial. One could question why this interval is chosen not other.
- Here one has two possible ways of treating such functions within the framework of Hilbert spaces:
 - either limit oneself to the functions that are square integrable over the entire line
 - or consider a weighted inner product that decrease effects of the functional tails.

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• Here we only announce an example of the second approach, which leads to an interesting little theory.

Data - Vectors or Functions	Vectors	Functions	Popular functional bases

The weighted inner product and Gaussian random variable

By L^Φ₂, we denote the Hilbert space of square integrable functions on ℝ with respect the Gaussian measure Φ(dx) = φ(x)dx, where φ(x) = e^{-x²/2}/√2π so the inner product of f, g ∈ L^φ₂ is given by

$$\langle f,g\rangle_{\phi}=\int_{\mathbb{R}}f(x)g(x)\phi(x)\,dx.$$

Let Z be a standard normal variable, then for f ∈ L₂^Φ the random variable f(Z) is has finite second moment and the set of all random variables of such form constitutes a closed subspace of L₂ that is isomorphic to L₂^Φ, where isomorphism is given by

$$\mathbb{E}(f(Z)g(Z)) = \langle f,g \rangle_{\phi}.$$

Since all moments of a standard normal random variable are finite, all polynomials are in \mathbb{L}_2^{Φ} . Moreover, they constitute a dense linear subspace of L_2^{Φ} . Recall the formula for the moments of the standard normal distribution

$$\mathbb{E}Z^{2k}=\frac{(2k)!}{2^kk!}.$$

Consequently, $M_k(x) = \sqrt{2^k k! / (2k)!} z^k$'s form normalized basis in L_2^{Φ} .

Definition

The Hermite polynomials H_k , $k \in \mathbb{N}_0$ are the orthonormal elements in L_2^{Φ} obtained by the Gram-Schmidt orthonormalization procedure applied to M_k , $k \in \mathbb{N}_0$.



Bases of polynomials – Hermite polynomials

Since the Gram-Schmidt orthonormalization produces H_N as a linear combination of M_k , k = 0, 1, ..., N thus H_N is a polynomial of order N and it is orthogonal to M_k , $k = 0, 1, \ldots, N - 1$.

The first six Hermite polynomials:

$$\begin{aligned} H_0(x) &= 1, \\ H_1(x) &= x, \\ H_2(x) &= (x^2 - 1)/\sqrt{2}, \\ H_3(x) &= (x^3 - 3x)/\sqrt{6}, \\ H_4(x) &= (x^4 - 6x^2 + 3)/\sqrt{24}, \\ H_5(x) &= (x^5 - 10x^3 + 15x)/\sqrt{120}. \end{aligned}$$

• Notice that H_{2k} are having only even powers of x while H_{2k+1} are having only odd numbered ones, it follows, for example from the next slide.

Data - Vectors or Functions	Vectors	Functions	Popular functional bases
Bases of polynomials –	Hermite polvno	mials	

• Let $P_n(x) = H_n(x)/\alpha_n$, where α_n is the coefficient of H_n at x^n . The polynomials P_n 's are referred to as the un-normalized Hermite polynomials. We note the following convenient representation of P_n and H_n .

Theorem

The Hermite polynomials are of the form

$$P_{n}(x) = (-1)^{n} e^{x^{2}/2} \frac{d^{n}}{dx^{n}} \left(e^{-x^{2}/2} \right)$$

$$H_{n}(x) = \frac{(-1)^{n}}{\sqrt{n!}} e^{x^{2}/2} \frac{d^{n}}{dx^{n}} \left(e^{-x^{2}/2} \right)$$
(2)

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We have also an explicit form the Hermit polynomials as given in

$$P_n(x) = n! \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(-1)^k}{2^{2k}} \frac{x^{n-2k}}{(n-2k)!k!}.$$