Documentation on the java^{TM} packet
Vector Fields

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Abstract

This documentation describes the usage and functionality of a Mathematica Notebook[1] for orthogonal functions. Sine and cosine functions may be selected as well as Legendre and Hermite polynomials.
This Notebook is an improvement of the orthogonal functions Notebook of the Demonstrations project by Alain Goriely and will be provided within the „OWL-project“„e-Module zur Veranschaulichung der Theoretischen Physik“on the web page of the „Institut für Theoretische Physik“[2]

[1]Mathematica is a registered trademark of Wolfram Research Inc. http://www.wolfram.com
[2]Translated to english by Stanislav Ax 31.03.2014

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Imprint

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Project: Offensive Wissen durch Lernen
e-Module zur Veranschaulichung der Theoretischen Physik
Head of the project: *Prof. Dr. Eckehard Schöll, PhD*
Contact: owl@itp.physik.tu-berlin.de

1 Introduction

The Mathematica Notebook illustrates the behavior of orthogonal functions out of three groups[3] in two two-dimensional plots. The Notebook presents two selected functions and their partial integrations next to each other.

Visualizatons that this applet may provide

- Legendre polynomials
- Hermite polynomials
- Sine- and cosine functions
- Their product functions and integration
- Various integration borders and weighting functions
- Various orders of the used functions

Visualizatons that this applet may not provide

- Automatic adjustment of the integration borders to the used functions
- Recognizing of analytically exact solutions(only numerical integration)
- Arbitrary high orders

2 Program

The program is a Mathematica Player^{TM} Notebook which can be used with the for free available Mathematica Player as well as with the commercial version of Mathematica 6. After the start, the initialization of Mathematica and the confirmation of the dynamical elements the start window will appear.

[3] In the source code further polynomials like the Chebyshev polynomial are commented

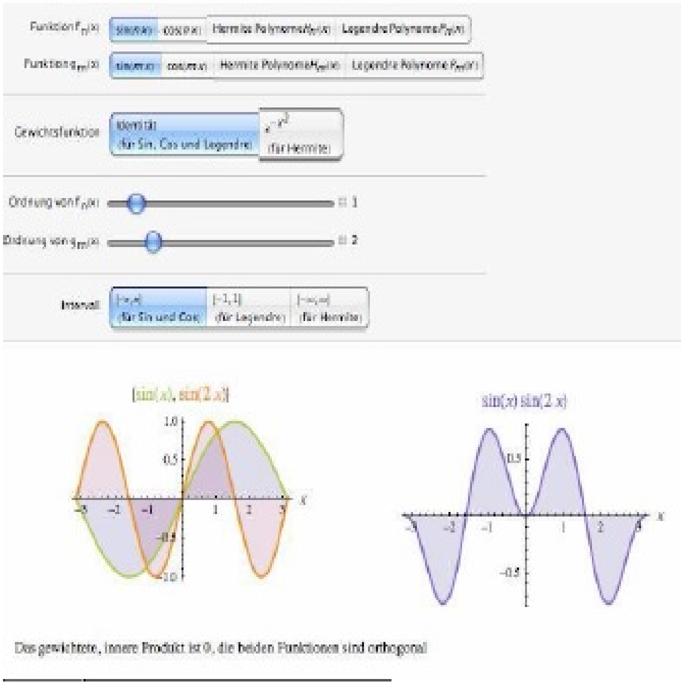

Figure 1: notebook right after the start

The program is using dynamical elements which are available since the introduction of Mathematica 6. This has to be confirmed with „Enable Dynamics“during the start of the program.

2.1 Program structure

The upper four rows are for selecting the functions and their orders. The functions have to be multiplicated with a corresponding weighting function in order to obtain the right integration. This weighting function is given by f(x)=1 for the sine function, the cosine function and the Legendre polynomials. In contrary for the Hermite polynomials a gauss function has to be used $f(x) = e^{-x^2}$. This is also valid for the integration borders which are amounting $[-\pi, \pi]$ for sine- and cosine functions, $[-1, 1]$ for Legendre polynomials and $[-\inf, \inf]$ for Hermite polynomials. If the weighting and borders are adjusted correct then the orthogonality of the functions can be checked with the two sliders.

Imaging area

The left frame is showing the two chosen functions. The right frame is for indicating the product of the functions. The area that this chart is enclosing within the corresponding borders together with the x-axis corresponds to the integral. The value of the integral is indicated under the both frames. If this value is equal to zero then the functions are called orthogonal.

2.2 Utilization

The orthogonality is checked here for functions out of one function system only. Hence the integration of different function kinds is not sensible as well as the choice of non suiting weighting functions and integration borders. A bigger area may be selected to estimate the behavior of the functions and their product outside of the borders. In this case the value of the integral is meaningless.

2.2.1 Manipulation of the source code

To expand the functionality of the Notebook a commercial version of Mathematica 6 has to be used. The source code becomes visible and editable Through the graphical part then.

2.3 Owner

The program is based on a version made by Alain Goriely and is available under the title *Orthogonality of Two Functions with Weighted Inner Product* in the *Wolfram Demonstrations Project*[4]

2.4 Technical requirements

A working version of the Mathematica Player or a commercial (It exists for Windows, Linux and Mac OS X) version of Mathematica 6 or higher has to be installed on the computer. The calculations may cause much calculational effort or occupy much heap space for high orders. Hence it is recommended to run the Mathematica Notebook on a computer with at least 800 MHz and 128 MB RAM. The monitors resolution should be set to at least 800×600 and at least 16.6 million colors should be supported.

3 Theory

The definition of the orthogonality of vectors in a supscpace of $\mathbb{R}^{\inf}$ is containing the scalar product. If the product yields zero (for example if two out of the three unit vectors are perpendicular to each other) then the projection is equal to zero as well. An implication is that they now can be varied independent of each other.

$$< f, g >= 0 \leftrightarrow f \perp g \tag{1}$$

For several vectors an orthogonal vector quantity is definable if each element is fulfilling the upper condition pairwise. Applying this to the function space in which the elements are continously differentiable functions then the scalar product is the integration of the product. The integration borders have to be chosen $[-\inf, \inf]$ if the continous differentiable function obtains an infinitely large domain.

[4] http://demonstrations.wolfram.com/OrthogonalityOfTwoFunctionsWithWeightedInnerProducts/

$$< f,g >= 0\int_{-\infty}^{\infty} dx f(x)g(x) \tag{2}$$

3.1 Sine and cosine

The Hilbert space is limited. All functions of the form f(x)=sin(nx) are for example orthogonal for two different $n \in \mathbb{N}$ (same is valid for cos). An arbitrary number of new functions may be generated by summation and multiplication of the base functions. The generated functions are often solutions for problems which are described by differential equations.

3.2 Legendre polynomials

This way for example the Legendre differential equation is solving the Laplace equation in spherical coordinates which describes the electrical field as Poisson equation. The variable is the cosine of an angle out of the spherical coordinates (r, ϑ, ϕ) . The Legendre differential equation is given by

$$(1 - x^2)y''(x) - 2x'(x) + \lambda y(x) = 0 \tag{3}$$

If this formulation is formulated as an eigenvalue problem then the eigenvalue λ may be expressed in the form l(l+1). The corresponding eigenfunctions are the Legendre polynomials P_l. According to the formula of Rodrigues one obtains the P_l by derivation of a function.

$$P(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l (x^2 - 1)^l} (l \geq 0, l) \tag{4}$$

3.3 Hermite polynomials

The Hermitian differential equation

$$y''(x) - 2xy'(x) + 2ny(x) = 0 \; n \in N \tag{5}$$

is solving the quantum mechanical harmonical oscillator

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) + \frac{1}{2} m\omega^2 x^2 \Psi(x) = E\Psi(x) \tag{6}$$

With the general ansatz for the Schrödinger wave Ψ

$$\Psi(x) = e^{-\frac{1}{2}z^2} v(z) \tag{7}$$

one obtains the following differential equation

$$v'' - 2zv' + (\frac{2E}{\hbar\omega} - 1)v = 0 \tag{8}$$

The comparence with the general Hermitian differential equation will lead to the known solutions for the equidistant energy values of the harmonical oscillator

$$2n = \frac{2E - 1}{\hbar\omega} \implies E_n = \hbar\omega(n + \frac{1}{2}) \tag{9}$$

The eigen functions of the equidistant energies are the Hermitian polynomials of the n-th order.

A Quelltexte

Das konvertieren eines Mathematica Player Notebooks (.nbp) aus einem normalen Notebook (.nb) ist ausschließlich über die Wolfram Webseite möglich. Daher ist hier die manipulierbare Notebook Variante des Programms mit identischer Funktion aufgelistet.

Listing 1: Mathematica Notebook Quellcode

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(* http://www.wolfram.com/nb *)

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B Literatur

Literatur

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