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Phys 331 - Numerical Techniques for the Sciences I.

Midterm 2

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(1) Orthogonalization [30 points]

Given the following three functions

$$\psi_1(x) = e^{-x}, \quad (1)$$
$$\psi_2(x) = e^{-2x}, \quad (2)$$
$$\psi_3(x) = e^{-3x}, \quad (3)$$

(1a) [5 pts] Are they orthogonal in the sense of the scalar product

$$(f,g) = \int_0^\infty f(x)g(x)dx \ ? \quad (4)$$

(Explain).

① $\langle \varphi_i, \varphi_j \rangle = \int_0^\infty e^{-ix} e^{-jx} dx = \int_0^\infty e^{-(i+j)x} dx$
for $\varphi_i = e^{-ix}$ and $\varphi_j = e^{-jx}$

② for $i \neq j$
$\langle \varphi_i, \varphi_j \rangle = \left. \frac{e^{-(i+j)x}}{-(i+j)} \right|_0^\infty = \frac{1}{i+j}$

③ for $i = j$ $\langle \varphi_i, \varphi_j \rangle = \frac{1}{2i}$

④ so $\langle \varphi_1, \varphi_2 \rangle = \frac{1}{1+2} = \frac{1}{3} \neq 0$ so φ_1, φ_2 are not orthogonal

⑤ $\langle \varphi_1, \varphi_3 \rangle = \frac{1}{1+3} = \frac{1}{4} \neq 0$ so φ_1, φ_3 are not orthogonal

⑥ $\langle \varphi_2, \varphi_3 \rangle = \frac{1}{2+3} = \frac{1}{5} \neq 0$
φ_2 and φ_3 are not orthogonal

⑦ so the functions are not orthogonal on interval $[0, \infty)$ w/ respect to the standard scalar product as shown above

(1b) [15 pts] Using the Gram-Schmidt process, obtain two new functions $\tilde{\psi}_1$ and $\tilde{\psi}_2$ by orthogonalizing ψ_1 and ψ_2 using the scalar product of part 1b.

① $\tilde{\varphi}_1 = \frac{\varphi_1}{\|\varphi_1\|}$

② $\|\varphi_1\|^2 = \langle \varphi_1, \varphi_1 \rangle = \int_0^\infty e^{-2x} dx = \frac{1}{2}$

③ $\|\varphi_1\|^2 = \frac{1}{\sqrt{2}}$

$\tilde{\varphi}_1 = \sqrt{2}\, e^{-x}$

④ To make φ_2 orthogonal to $\tilde{\varphi}_1$, we substract the projection of φ_2 onto $\tilde{\varphi}_1$

⑤ $\hat{\varphi}_2 = \varphi_2 - \langle \varphi_2, \tilde{\varphi}_1 \rangle \hat{\varphi}_1$

⑥ $\langle \varphi_2, \tilde{\varphi}_1 \rangle = \sqrt{2} \int_0^\infty e^{-2x} e^{-x} dx = \sqrt{2} \int_0^\infty e^{-3x} dx = \frac{\sqrt{2}}{3}$

⑦ $\langle \varphi_2, \tilde{\varphi}_1 \rangle \tilde{\varphi}_1 = \frac{2}{3} e^{-x}$

⑧ $\tilde{\varphi}_2 = \varphi_2 - \frac{2}{3} e^{-x} = e^{-2x} - \frac{2}{3} e^{-x}$

⑨ Normalize $\hat{\varphi}_2$

⑩ $\|\tilde{\varphi}_2\|^2 = \langle \tilde{\varphi}_2, \tilde{\varphi}_2 \rangle$, $\tilde{\varphi}_2 = e^{-2x} - \frac{2}{3} e^{-x}$
$\langle \tilde{\varphi}_2, \tilde{\varphi}_2 \rangle = \int_0^\infty (e^{-2x} - \frac{2}{3} e^{-x})^2 dx$
$= \frac{1}{4} - \frac{4}{3} \cdot \frac{1}{3} + \frac{4}{9} \cdot \frac{1}{2} = \frac{1}{36}$

⑪ $\|\tilde{\varphi}_2\| = \frac{1}{6}$

⑫ $\tilde{\varphi}_2 = 6(e^{-2x} - \frac{2}{3} e^{-x})$
$\tilde{\varphi}_2 = 6e^{-2x} - 4e^{-x}$

⑬ $\boxed{\tilde{\varphi}_1 = \sqrt{2}\, e^{-x} \qquad \tilde{\varphi}_2 = 6e^{-2x} - 4e^{-x}}$

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(1c) [5 pts] Write down (but don't evaluate) what the last orthogonal vector $\tilde{\psi}_3$ would look like. You may leave your inner products as (f,g).

① $\tilde{\varphi}_3 = \varphi_3 - \frac{(\varphi_3, \tilde{\varphi}_1)}{(\tilde{\varphi}_1, \tilde{\varphi}_1)}\tilde{\varphi}_1 - \frac{(\varphi_3, \tilde{\varphi}_2)}{(\tilde{\varphi}_2, \tilde{\varphi}_2)}\tilde{\varphi}_2$

⑤ substitute

$\tilde{\varphi}_3 = e^{-3x} - \frac{(\varphi_3, \tilde{\varphi}_1)}{1}\sqrt{2}e^{-x} - \frac{(\varphi_3, \tilde{\varphi}_2)}{1/36}(6e^{-2x} - 4e^{-x})$

② $(\varphi_3, \tilde{\varphi}_1) = \int_0^\infty \varphi_3(x)\tilde{\varphi}_1(x)\,dx$

③ $(\varphi_3, \tilde{\varphi}_2) = \int_0^\infty \varphi_3(x)\tilde{\varphi}_2(x)\,dx$

④ $(\tilde{\varphi}_1, \tilde{\varphi}_1)$ and $(\tilde{\varphi}_2, \tilde{\varphi}_2)$ are norms of $\tilde{\varphi}_1$ and $\tilde{\varphi}_2$ → already known ⇒ $\tilde{\varphi}_1 = \sqrt{2}e^{-x}$ $\tilde{\varphi}_2 = 6e^{-2x} - 4e^{-x}$

(1d) [5 pts] Let's say I wanted to extend my inner product to go from $-\infty$ to ∞. Describe one modifiation you could make to the inner product above to make sure the integrals converge.

we can introduce a weight function $w(x)$ that decays rapidly as $|x| \to \infty$ so

$$\langle f, g \rangle = \int_{-\infty}^{\infty} f(x)g(x)w(x)\,dx.$$

This weight function can be the gaussian function $w(x) = e^{-x^2}$ b/c it decay exponentially as $|x| \to \infty$ and ensures that the product $f(x)g(x)w(x)$ vanishes at both ends. This guarentees that the integrals of functions like e^{-ax} over $(-\infty, \infty)$ converge.

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$(1-\lambda)(-1-\lambda)-4$

$-1-\lambda+\lambda+\lambda-4$

(1) The Eigenproblem [20 points]

(2a) [15] Calculate the eigenvectors and eigenvalues of

$$\mathbf{T} = \begin{pmatrix} 1 & 2 \\ 2 & -1 \end{pmatrix}$$

(5)

① char eqn

$\det(T-\lambda I)=0$

$T-\lambda I = \begin{pmatrix} 1-\lambda & 2 \\ 2 & -1-\lambda \end{pmatrix}$

$\det(T-\lambda I) = (1-\lambda)(-1-\lambda)-(2)(2)$

$= \lambda^2 \cancel{-2\lambda} - 5 \Rightarrow \boxed{\lambda = \pm\sqrt{5}}$

$\lambda = \cancel{\frac{-(-1)\pm\sqrt{(-1)^2-4(1)(-5)}}{2(1)}} = \cancel{\frac{1\pm\sqrt{21}}{2}}$

$\cancel{\lambda_1 = \frac{1+\sqrt{21}}{2} \quad \lambda_2 = \frac{1-\sqrt{21}}{2}}$

eigenvalues

Eigenvectors:

~~② solve $(T-\lambda I)v = 0$ for some eigenvector v~~

~~λ_1: $T-\lambda_1 I = \begin{pmatrix} 1-\frac{1+\sqrt{21}}{2} & 2 \\ 2 & -1-\frac{1+\sqrt{21}}{2} \end{pmatrix}$~~

~~let $v = \binom{x}{y}$~~

~~$\frac{1-\sqrt{21}}{2}x + 2y = 0 \Rightarrow y = -\frac{1-\sqrt{21}}{4}dx$~~

~~$2x - \frac{1+\sqrt{21}}{2}y = 0$~~

~~$\boxed{V_1 = \begin{pmatrix} 1 \\ -\frac{1-\sqrt{21}}{4} \end{pmatrix} \text{ for } \lambda_1}$~~

~~λ_2: $T-\lambda_2 I = \begin{pmatrix} 1-\frac{1-\sqrt{21}}{2} & 2 \\ 2 & -\frac{1-\sqrt{21}}{2} \end{pmatrix}$~~

~~$\frac{(1+\sqrt{21})x}{2} + 2y = 0 \Rightarrow y = -\frac{1+\sqrt{21}}{4}x$~~

~~$2x - \left(\frac{1-\sqrt{21}}{4}\right) = 0$~~

~~$\boxed{V_2 = \begin{pmatrix} 1 \\ -\frac{1+\sqrt{21}}{4} \end{pmatrix} \text{ for } \lambda_2}$~~

(2b) [5 pts] I can diagionalize a matric with $\mathbf{U}^{-1}\mathbf{TU} = \mathbf{D}$. What are the matricies **U** and **D** in this case?

$\lambda_1 = \sqrt{5}$

$T-\lambda I = \begin{bmatrix} 1-\sqrt{5} & 2 \\ 2 & -1-\sqrt{5} \end{bmatrix}$

$v = \begin{bmatrix} x \\ y \end{bmatrix}$

$\begin{bmatrix} 1-\sqrt{5} & 2 \\ 2 & -1-\sqrt{5} \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$

$\vec{v}_1 = \begin{bmatrix} 1 \\ -\frac{1-\sqrt{5}}{2} \end{bmatrix}$ for $\lambda_1 = \sqrt{5}$

$\vec{v}_2 = \begin{bmatrix} 1 \\ -\frac{1+\sqrt{5}}{2} \end{bmatrix}$ for $\lambda_2 = -\sqrt{5}$

$U = \begin{bmatrix} 1 & 1 \\ -\frac{1-\sqrt{5}}{2} & -\frac{1+\sqrt{5}}{2} \end{bmatrix}$

$D = \begin{bmatrix} \sqrt{5} & 0 \\ 0 & \sqrt{5} \end{bmatrix}$

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(3) Linear operators [25 points]

(3a) [13 pts] - Calculate the matrix elements of the operator

$$D = \frac{d^2}{dx^2} \tag{6}$$

in the basis $Z = \{\psi_1, \psi_2, \psi_3, \psi_4\}$, where

$$\psi_1 = e^x + e^{-x} \tag{7}$$
$$\psi_2 = e^x - e^{-x} \tag{8}$$
$$\psi_3 = e^x \tag{9}$$
$$\psi_4 = e^{-2x} \tag{10}$$

$D\psi = \frac{d^2\psi}{dx^2}$ $\quad D_{ij} = \langle \psi_{i}, \frac{d^2\psi_j}{dx^2} \rangle$

$\frac{d^2\psi_1}{dx^2} = \frac{d^2}{dx^2}(e^x + e^{-x}) = e^x + e^{-x}$

$\frac{d^2\psi_2}{dx^2} = e^x - e^{-x}$

$\frac{d^2\psi_3}{dx^2} = e^x$

$\frac{d^2\psi_4}{dx^2} = 4e^{-2x}$

$D\psi_1 = \psi_1$
$D\psi_2 = \psi_2$
$D\psi_3 = \psi_3$
$D\psi_4 = 4\psi_4$

So in basis $Z = \{\psi_1, \psi_2, \psi_3, \psi_4\}$

$$\boxed{D = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix}}$$

(3b) [7 pts] - Within the vector space spanned by the basis Z, calculate the kernel of D. **Hint:** Find which linear combinations of the ψ_k give zero when D is applied to them.

$D(c_1\psi_1 + c_2\psi_2 + c_3\psi_3 + c_4\psi_4) = 0$

$\Downarrow$

$c_1 D\psi_1 + c_2 D\psi_2 + c_3 D\psi_3 + c_4 D\psi_4$

$\Downarrow$

$c_1\psi_1 + c_2\psi_2 + c_3\psi_3 + 4c_4\psi_4 = 0$

$c_1 = 0 \quad c_3 = 0$

$c_2 = 0 \quad 4c_4 = 0 \Rightarrow c_4 = 0$

so $c_1 = c_2 = c_3 = c_4 = 0$

$Ker(D) = \{0\}$

3c [5 pts] - Is the operator D invertible in the space spanned by the basis Z? Is your answer consistent with your answer to the previous question? Explain.

An operator is invertible if and only if it its kernal is trivial (contains only the $\vec{0}$)

$Ker(D) = \{0\} \Rightarrow D$ is injective / one to one

the vector space spanned by Z is 4D b/c $Z = \{\psi_1, \dots, \psi_4\}$ is a basis. The range of D is also a subspace of the same 4D space, since D is injective and operates w/i a finite dim vector space, it must be surjective (onto). This implies D is bijective.

so it is invertible. our previous answer is consistency.

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(4) Fourier Series [25 points]

For this problem we will use a version of the Fourier series starting at $x_0 = 0$ with $L = 2\pi$:

$$f(x) = \frac{A_0}{2} + \sum_{k=1}^{\infty} \left[A_k \cos(kx) + B_k \sin(kx)\right] \tag{11}$$

where

$$A_k = \frac{1}{\pi}\int_0^{2\pi} f(x)\cos(kx)\,dx \quad \text{and} \quad B_k = \frac{1}{\pi}\int_0^{2\pi} f(x)\sin(kx)\,dx \tag{12}$$

(4a) [10 pts] Starting with the function

$$f(x) = e^{ix} + e^{i3x} \tag{13}$$

Compute all non-zero A_k and B_k.

$f(x) = (\cos(x) + \cos(3x)) + i(\sin(x) + \sin(3x))$

$Re[f(x)] = \cos x + \cos 3x$

$Im[f(x)] = \sin x + \sin 3x$

$A_k = \frac{1}{\pi}\int_0^{2\pi} f(x)\cos(kx)dx$

$f(x) = \cos(x)$

$\frac{1}{\pi}\int_0^{2\pi} \cos(x)\cos(kx)dx = \begin{cases} 1 & \text{if } k=1 \\ 0 & \text{otherwise} \end{cases}$

$f(x) = \cos(3x)$

$\frac{1}{\pi}\int_0^{2\pi} \cos(3x)\cos(kx)dx = \begin{cases} 1 & \text{if } k=3 \\ 0 & \text{otherwise} \end{cases}$

so $A_k = \begin{cases} 1 & \text{if } k=1 \text{ or } k=3 \\ 0 & \text{otherwise} \end{cases}$

(4b) [10 pts] It would be more natural to express this quantity using the complex version of the Fourier series

$$f(x) = \sum_{k=-\infty}^{\infty} C_k e^{ikx} \quad \text{where} \quad C_k = \frac{1}{2\pi}\int_0^{2\pi} f(x)e^{-ikx}dx \tag{14}$$

With the same function as above, compute all non-zero C_k.

didn't finish no time :(

$B_k = \frac{1}{\pi}\int_0^{2\pi} f(x)\sin(kx)dx$

$f(x) = \sin(x)$

$\frac{1}{\pi}\int_0^{2\pi} \sin(x)\sin(kx)dx = \begin{cases} 1 & \text{if } k=1 \\ 0 & \text{otherwise} \end{cases}$

$f(x) = \sin(3x)$

$\frac{1}{\pi}\int_0^{2\pi} \sin(3x)\sin(kx) = \begin{cases} 1 & \text{is } k=3 \\ 0 & \text{otherwiser} \end{cases}$

$\rightarrow B_k = \begin{cases} 1 & \text{if } k=1 \text{ or } k=3 \\ 0 & \text{otherwise} \end{cases}$

$A_1 = 1$

$A_3 = 1$

$B_1 = 1$

$B_3 = 1$

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(4c) [5 pts] Instead of the above function, say I was trying to fit a non-periodic function (e.g. $f(x) = x$) with a Fourier series over the interval $[0, 2\pi]$. What would this look like? Sketch your answer.