MADS-CLAUSEN-INSTITUTE, SDU
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Computational Physics: Problem Set 1

Discussion: 01/02/2023

1 Matrix algebra

Consider the 2×2-matrices $A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $B = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $C = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $D = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

a) Compute the matrices $E = \frac{1}{2}(5A - 3B + 5C - D)$, $\quad F = (B + C)E$

b) Find the eigenvalues of A, B, C and F. Show that D has no real eigenvalues.
Which matrices have degenerate eigenvalues?
hint: not every case requires a calculation, some are trivial.

c) Find all eigenvectors of A, B, C and F.
hint: not every case requires a calculation, some are trivial.

d) Matrix multiplication is not commutative (i.e. the order of the factors can matter). The commutator of two matrices is defined as $[M_1, M_2] = M_1 M_2 - M_2 M_1$.
Calculate the commutators $[A, B]$, $\quad [A, C]$, $\quad [C, D]$, $\quad$ and $[E, F]$.
Which of these pairs of matrices do commute?

2 Hilbert space of complex column vectors

Let $\mathbb{C}^N$ be the space of complex column vectors

$$\mathbb{C}^N = \{\mathbf{a} : \mathbf{a} = (a_1, \ldots, a_N)^T \quad \text{with} \quad a_n \in \mathbb{C}\},$$

defined over the field of complex numbers $\mathbb{C}$ with the usual scaling and addition:

$$\alpha\mathbf{a} + \beta\mathbf{b} = (\alpha a_1 + \beta b_1, \ldots, \alpha a_N + \beta b_N), \quad \text{with} \quad \mathbf{a}, \mathbf{b} \in \mathbb{C}^N, \quad \alpha, \beta \in \mathbb{C}.$$

a) Show that $\mathbb{C}^N$ is complete by assuming that $\mathbb{C}$ is complete.

b) Show that the scalar product

$$\langle \mathbf{a}, \mathbf{b} \rangle = \sum_{i=1}^{N} a_i^* b_i$$

is Hermitian, positive definite, and linear in the second parameter.

c) Show that the matrix $M_{ij}^{(\Phi)}$ associated with a Hermitian automorphism Φ acting on $\mathbb{C}^N$, i.e. the matrix representing Φ with

$$\langle \Phi(\mathbf{a}), \mathbf{b} \rangle = \langle \mathbf{a}, \Phi(\mathbf{b}) \rangle \quad \text{for} \quad \mathbf{a}, \mathbf{b} \in \mathbb{C}^N$$

satisfies the condition

$$M_{ji}^{(\Phi)} = [M_{ij}^{(\Phi)}]^*.$$

$\boxed{3}$ Hilbert space of polynomials of degree N

A polynomial of degree N takes the form $p(x) = a_0 + a_1 x + a_2 x^2 + \ldots a_N x^N = \sum_{n=0}^{N} a_n x^n$ and is completely definied via its coefficients $a_n \in \mathbb{R}$. All polynomials of degree N form a *function space* $\mathbb{P}$. We now define the space $\mathbb{R}^{N+1}$ of column vectors $(a_0, a_1, \ldots a_N)^T$ and write $\mathbf{V}[p(x)]$ for the column vector that consists of the coefficients of the polynomial $p(x)$.

a) Show that the spaces $\mathbb{P}$ and $\mathbb{R}^{N+1}$ follow the same calculation rules for addition and scaling:

$$\mathbf{V}[\lambda p(x) + \mu q(x)] = \lambda \mathbf{V}[p(x)] + \mu \mathbf{V}[q(x)] \quad \text{for} \quad p, q \in \mathbb{P}, \quad \lambda, \mu \in \mathbb{R}.$$

b) Show that the derivative $\frac{\mathrm{d}}{\mathrm{d}x}$ of an element of $\mathbb{P}$ always produces another element from $\mathbb{P}$, i.e. that the derivative $\frac{\mathrm{d}}{\mathrm{d}x}$ constitutes an automorphism. Show that the action of the derivative $\frac{\mathrm{d}}{\mathrm{d}x}$ on the polynomials from $\mathbb{P}$ can be represented as a matrix within the space $\mathbb{R}^{N+1}$ and find this matrix.

c) Show that the action of the integral $\int_0^x \mathrm{d}x'\, p(x')$ (i.e. the inverse operation of the derivative) on the polynomials $p(x)$ from $\mathbb{P}$ **cannot** be represented as a matrix within the space $\mathbb{R}^{N+1}$.

d) Show that the evaluation of any polynomial $p(x) \in \mathbb{P}$ at a given position x_0 can be found by multiplying $\mathbf{V}[p(x)]$ with an appropriate vector of length $N+1$.

e) Show that the form

$$\langle p(x), q(x) \rangle = \int_0^1 \mathrm{d}x \; p(x) q(x) \quad \text{for} \quad p, q \in \mathbb{P},$$

is Hermitian, positive definite, and linear in the second parameter. Note that the Hermiticity condition simplifies to $\langle p, q \rangle = \langle q, p \rangle$, because the functions are purely real.

f) Show that the space $\mathbb{P}$ of polynomials of degree N is complete.

Students are encouraged to solve these problems in groups. They should be able to informally present their solution in the problem class on 01/02/2023 at the white board (no PowerPoint slides to be prepared).