

Lecture 5: Operators

Filipp Furche

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<http://ffgroup.chem.uci.edu>

Vector Spaces

A set E is called vector space (linear space) over a field \mathbb{K} iff

$\forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in E, \forall a, b \in \mathbb{K},$

1. vector addition “+” is defined, and E is an Abelian group with vector addition as composition law.
2. multiplication with scalars is defined, i.e., $a\mathbf{x} \in E$, and
 - (i) $a(b\mathbf{x}) = (ab)\mathbf{x}$
 - (ii) $(a + b)(\mathbf{x}) = a\mathbf{x} + b\mathbf{x}$
 - (iii) $a(\mathbf{x} + \mathbf{y}) = a\mathbf{x} + a\mathbf{y}$
 - (iv) $1\mathbf{x} = \mathbf{x}$

Examples of Vector Spaces

- \mathbb{R}^n over \mathbb{R} , \mathbb{C}^n over \mathbb{C} , e.g. “real (position) space”, reciprocal (momentum) space, phase space, etc.
- Normal modes of a molecule, lattice vibrations
- Hilbert space, e.g., space of all molecular orbitals, spin space

Inner and Outer Products in \mathbb{R}^n

- Inner product: Bilinear, positive definite map $\mathbb{R}^n \rightarrow \mathbb{R}$ s.t.
 $\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^n$

$$(\mathbf{x}|\mathbf{y}) = \mathbf{x} \cdot \mathbf{y} = \mathbf{x}^T \mathbf{y} = \sum_{i=1}^n x_i y_i$$

- Induces “Euclidean” norm $\|\mathbf{x}\| = |\mathbf{x}| = \sqrt{\mathbf{x} \cdot \mathbf{x}}$
- Example: Scalar product of two 3-vectors
- Outer (tensor) product: Bilinear map $\mathbb{R}^n \rightarrow \mathbb{R}^{n \times n}$ s.t.

$$\mathbf{x} \otimes \mathbf{y} = \mathbf{xy}^T = \begin{pmatrix} x_1 y_1 & x_1 y_2 & \cdots \\ x_2 y_1 & x_2 y_2 & \cdots \\ \vdots & \ddots & \cdots \end{pmatrix}$$

- Neither of these products qualify for group multiplication

Operator Algebras

- A linear operator $\mathbf{A} : E \rightarrow E$ is a linear map of a vector space E onto itself.
- Linear operators on \mathbb{R}^n are real $n \times n$ matrices.
- A linear operator is itself an element of another vector space $E \otimes E$, because addition and scalar multiplication are defined. For example, $\mathbb{R}^{n \times n}$ is a vector space with respect to addition of matrices and their multiplication by scalars.
- Multiplication of operators $\mathbf{A}, \mathbf{B} \in E$ is defined as bilinear map on $E \otimes E$ such that \mathbf{AB} is the operator corresponding to \mathbf{B} followed by \mathbf{A} . For example, for two matrices $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{n \times n}$,

$$\mathbf{A} \cdot \mathbf{B} = \mathbf{A}^T \mathbf{B}$$

(matrix multiplication)

- Vector spaces with bilinear maps are “algebras”.