

A SHORTNOTE ON APPLICATIONS OF MATHEMATICS

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Abstract

The scientific explanation of any theory may trace its roots to some branch of mathematics. A complete survey of applications of mathematics in other branches of science may require more than a human lifespan. This paper is an attempt to discuss some applications of mathematics in chemistry and physics. Algebraic methods and algebraic structures are commonly used in chemistry while integration, differential equations and their solutions are commonly used in physics.

Keywords: Algebraic structures, Representations, Symmetry.

Introduction

Mathematics is known as the queen of sciences. It is because the study of any branch of science involves the use of mathematics in various forms. For this reason, a strong base of mathematics is essential for the study of any branch of science. The problems related to distance and time in physics are solved using algebraic methods. The velocity and acceleration of a particle are represented by vectors in 3-dimensional Euclidean space R^3 . The eigenvalues of a matrix are determined by solving the characteristic equation of the matrix, which has a lot of applications in spectral analysis. Similarly group theory is an essential part of chemistry to understand atomic structures and related topics.

Algebra has various applications in chemistry and physics. Algebra involves the study of structures on sets. A set is a well-defined collection of objects. A structure consists of one or more binary operations on the set, which obey certain rules, also called axioms. Addition is an example of a binary operation. There are a lot of basic algebraic structures such as monoid, semi group, group, ring, field, modules and vector spaces. Apart from this, a lot of algebraic structures are being defined based on these structures to fulfil particular needs from time to time. A clear understanding of algebraic structures requires understanding the basic facts and peculiarities of the domain in which we are working.

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dimensional Euclidean space R^3 . The eigenvalues of a matrix are determined by solving the characteristic equation of the matrix, which has a lot of applications in spectral analysis. Similarly chemistry and computer science uses algebraic methods excessively for solving various types of problems. For instance, determination of number of atoms in a chemical equation is done by solution of algebraic equations.

Dealing with symmetry

The concept of symmetry is very important in researches related to chemistry, physics and biology. Symmetry and asymmetry directly affect how molecules respond to light waves, form bonds and operate biologically. Group theory can provide methods to determine how symmetry of a molecule is related to physical properties of molecules, such as energy levels of the orbitals, transitions between energy levels and even details of bonds. The Cayley's Theorem [1] states that every group is the subgroup of some Symmetry group. That is, every group is a permutation group. This motivated the study of algebraic combinatorics. Group actions[2] are used to study symmetries or automorphisms of mathematical objects. Informally, a group action is a dynamical process on an object, which partitions its members into sets which we call orbits. The study of the structure and quantity of these orbits yields important combinatorial results. The Dihedral group is the automorphism group of the Cycle graph. A permutation is a one-to-one, onto function defined from a set A to itself. A permutation is actually a rearrangement of the elements. It is proved that the set of all permutations defined on a set forms a group, called the permutation group. There are $n!$ permutations defined on a set of n elements forming the symmetric group S_n . For example, if a set A has three elements, say $A = \{1, 2, 3\}$ then there are $3! = 6$ permutations. The Collection of these six elements are known as the group of symmetries of a triangle.

Symmetry has a very big role in the study of molecular chemistry. The identity operation (E) is leaving the molecule as it is. This is equivalent to any number of full rotations around any axis. Rotation around an axis (C_n) consists of rotating the molecule around a specific axis by a specific angle. For example, if a water molecule is rotated 180° around the axis, it is in the same configuration as it started. Other symmetry operations are: reflection, inversion and improper rotation (rotation followed by reflection). A symmetrical molecule is one whose appearance does not change if you turn it about an axis of symmetry. ie, original and rotated states are indistinguishable from one another.

Symmetry was studied mathematically with reference to crystal symmetry. If you rotate a crystal by certain angles about certain axes, or reflect it in certain planes, you find equivalent faces in equivalent places. The branch Spatial symmetry[7] deals with operations that keep one point fixed, which constitute point groups. The collection of symmetry operations form a group. For example, the Ammonia molecule (NH_3) is composed of one nitrogen atom and three hydrogen atoms has C_{3v} symmetry (which is isomorphic to the symmetric group S_3 of 6 elements) and all of the properties contained in the C_{3v} character table are relevant to an ammonia molecule. It is also estimated that the ammonia molecule has 6 vibrational transitions. Let us suppose that symmetry elements of ammonia molecule are $E, C_3, C_3^2, \sigma, \sigma', \sigma''$. If we denote the original symmetry plane by σ , then rotations carry this plane into equivalent symmetry planes σ' and σ'' . A general point P is carried into the other two solid points by rotations, and into the open points by reflections in the three symmetry planes. Now, we may consider interactions between the rotations and reflections in this group. Suppose we reflect P in σ , then rotate clockwise by C_3 , and finally reflect again in σ . The result is the same as rotating anticlockwise by C_3^2 . Algebraically, we can write $\sigma^{-1} C_3 \sigma = C_3^2$. The associated members of a group form a class. The members of same class are similar in nature. The algebraic approaches of quantum chemistry mainly uses two alternative algebraic structures: the fundamental group of reaction mechanisms, based on the energy-dependent topology of potential energy surfaces, and the interrelations among point symmetry groups for various distorted nuclear arrangements of molecules. These two, distinct algebraic structures provide interesting interrelations, which can be exploited in actual studies of molecular conformational and reaction processes.

In theoretical organic chemistry, the algebraic structure count is introduced as the difference between the number of even and odd Kekule structures (named after the famous German organic chemist August Kekule) [7] of a conjugated molecule. Precisely, algebraic structure count (ASC-value) of the bipartite graph G corresponding to the skeleton of a conjugated hydrocarbon is defined using the adjacency matrix of G . In the case of bipartite planar graphs containing only circuits of the length of the form $4s+2$ ($s=1,2,\dots$) (the case of benzenoid hydrocarbons), this number is equal to the number of the perfect matchings (K -value) of G . There are algebraic formulae due to Serbian chemist and mathematician Ivan Gutman for finding the algebraic structure count. The recurrence formula for number of perfect matchings is given by $K\{G\}=K\{G-e\}+K\{G-(e)\}$ where $(G-e)$ is the subgraph

obtained from the graph G by deleting the edge e and $G-(e)$ is the subgraph obtained from G by deleting both the edge e and its terminal vertices).

Applications of representation theory

Researchers in Physics use group representations [4] to obtain information from symmetries. Representations of a group are in some sense a concrete realization of the group in the form of matrices acting on a vector space. It allows certain members of the space to be created that are symmetrical, and which can be classified by their symmetry. It is found that all the observed spectroscopic states of atoms and molecules correspond to such symmetrical functions, and can be classified accordingly.

Algebraic structures has a lot of applications in other sciences. Among these, Groups are of prime importance. A Group [1] is a set together with an associative binary operation containing the identity element and inverses of each element. If the elements commute with respect to the operation, then it is called an abelian group and if all elements can be obtained by repeated application of a single element to itself, it is called a cyclic group. Almost all structures in abstract algebra may be considered as special cases of groups. For example, Rings[1] can be viewed as abelian groups with respect to addition together with a second operation multiplication. A Field[1] is an additive abelian group, while the non-zero elements of a field form a multiplicative group. Even a Vectorspace[1] is an abelian group, with the operation being addition. A Point Group describes all the symmetry operations that can be performed on a molecule that results in a conformation indistinguishable from the original. Point groups are used to determine properties such as a molecule's molecular orbitals. There are only two one-dimensional point groups, the identity group and the reflection group.

Vectorspaces as an abstract algebraic structure was first defined by the Italian mathematician Giuseppe Peano in 1888. The importance of vectorspaces is that nearly everything in mathematical modeling is a vector in one way or another, and frequently the vectorspace operations are to be applied. A Vectorspace(also called a linear space) is a collection of objects called vectors, which may be added together and multiplied by scalars. The operations of vector addition and scalar multiplication must satisfy the specified axioms. A subspace is a vector space inside a vector space. A plane through the origin of $\mathbb{R}^3$ forms a subspace of $\mathbb{R}^3$. This is evident geometrically as follows: Let W be any plane through the origin and let u and v be any vectors in W other than the zero vector. Then $u + v$ must lie in W because it is the diagonal of the parallelogram determined by u and v ,

and ku must lie in W for any scalar k because ku lies on a line through u . Thus, W is closed under addition and scalar multiplication, so it is a subspace of R^3 .

Let us now generate some representations of the group. We can set up rectangular coordinates x, y, z , perhaps with z along the symmetry axis and x along one of the symmetry planes, with y making a right-handed system. Then point P can be expressed as (x, y, z) . Any symmetry operation will take these coordinates into (x', y', z') which are linear functions of the original coordinates. Explicitly, the transformation can be expressed as 3×3 matrices acting on 3-dimensional column vectors. There will be six matrices, and E will correspond to the identity matrix. The matrices are easily found from the formulas for rotation of coordinates. We notice that z is not affected. It is multiplied by 1 in each transformation and the values of x, y are never mixed in. Therefore, z is the basis of a representation all by itself, the unit representation where each member corresponds to 1. The values of x and y do get mixed under the transformations, and it is easy to see that no choice of coordinates could ever change this. They form the basis of a two-dimensional matrix representation. The representation in terms of (x, y, z) is said to be reducible to the two smaller representations, and each of these is irreducible to smaller representations. It is the irreducible representations that give the essential information and a 1-dimensional representation is naturally irreducible.

Any representation changes its explicit form if we make a different choice of basis. Choosing a different basis is a linear transformation $y = Ax$, under which the matrices R of a representation change into $R' = A^{-1}RA$. This is called a similarity transformation[6]. The diagonal sum or trace of the matrix R is invariant under such a transformation and this trace is called the character of the member in the representation. If the characters of two representations are the same, then the representations are equivalent and two equivalent representations differ only in the choice of basis functions used to express them explicitly.

The characters of matrices representing the members of a class will be the same, as we know that the members of a class are related by similarity transformations. The number of irreducible representations of a group is equal to the number of classes. We can construct tables showing the characters of its irreducible representations. As an example, the states of an isolated atom are classified by the total angular momentum J , and belong to irreducible representations of the rotation group in three dimensions with dimension $2J + 1$. As long as there is spherical symmetry, these states all have exactly the same energy. When a magnetic

field is applied, then the $2J + 1$ levels now acquire different energies, and Group theory can determine these states in advance.

The electric dipole moment is a vector, and corresponds to the irreducible representation $J = 1$ of the rotation group. Operating on a state of angular momentum J , it gives representations corresponding to $J + 1$, J , and $J - 1$. The other state involved must have one of these values of J , or the result will not contain the unit representation $J = 0$. Therefore, we have the selection rule that J changes only by ± 1 or 0 in an electric dipole transition.

Lie groups[3] were introduced to model the continuous symmetries of differential equations, in the same way that finite groups are used in Galois theory[1] to model the discrete symmetries of algebraic equations. A Continuous group is a group having continuous group operations. The rotation group O_3 is an example of a continuous group. For O_3 , we could use the two angles specifying the orientation of the axis of rotation, and the angle of rotation about this axis. The Lie algebra expresses the structure of the group in a concise and usable form. The conservation of angular momentum is a consequence of the O_3 symmetry. In general, any continuous symmetry may be considered to be associated with a conservation law. Linear momentum is similarly related to symmetry under displacement of the system in space, and energy to displacement in time. Finite symmetries are not associated with conserved quantities. Two important symmetries in quantum mechanics are inversion symmetry or parity, and time reversal symmetry.

Applications of Algebra in Computer science

Discrete mathematics [9] and Boolean Algebra [8] form the foundation for Computer science and coding theory. Finite groups are used based on multiplication of integers in asymmetric encryption schemes [3] such as RSA (Rivest-Shamir-Adleman - algorithm used by modern computers to encrypt and decrypt messages) in cryptography. The error correction codes [3] like Reed-Solomon codes and Chinese remainder codes use the ideas of Rings and Ideals. Algebraic concepts and structures are used in algorithms and functions [5] in computer programming. For example, when the “%” remainder function is used, we are considering a cyclic group with respect to modulo operation.

Finite fields, especially Galois fields play a very important role in Computer science. A field F is an algebraic system with two operations, namely addition and multiplication. A field K is said to be an Extension Field of a field F , if F is a sub-field of K . For example, the field of Complex Numbers is an extension of the field of Real Numbers. A theorem due to

Kronecker [1] states that if F is a field and let $f(x)$ is a non-constant polynomial in $F[x]$, then there is an extension field E of F and an element α in E such that $f(\alpha) = 0$. If we have a finite field and an irreducible polynomial over the field, then we can construct a finite field using the root of the irreducible polynomial lying in an extension field. For example, $p(x) = x^2 + x + 1$ is irreducible over Z_2 . Then there is an extension field E of Z_2 containing a zero α of $p(x)$. Then $Z_2(\alpha) = \{b_0 + b_1\alpha \mid b_i \in Z_2\}$. That is, $Z_2(\alpha) = \{0, 1, \alpha, 1 + \alpha\}$. Thus we have a new finite field of four elements. The field of Complex numbers is algebraically closed. That is every non-constant polynomial $f(x)$ in $C[x]$ has a zero in C . We can construct a polynomial with real coefficients (for example $p(x) = x^2 + 1$) having no zero in R . But this is impossible in C . In other words C may be considered as complete or perfect.

Algebraic structures like semigroups and monoids are used excessively in automata theory and coding theory. Cayley Graphs [2] are used in designing communication architectures for parallel and distributed computation, in which each vertex represents a separate processor and each edge represents a communication link between two processors. Maximization of the number of processors given a fixed number of links per processor, finding effective transmission schemes that minimize traffic congestion are typical research topics. Polya enumeration theory [3] studies the number of distinct colourings or automorphisms of groups such as rotations of 3D objects. Constraint satisfaction problems involving homomorphisms of relational structures arise frequently in artificial intelligence which are solved using algebraic techniques.

Algebra and algebraic geometry are the basis of nearly all modern cryptographic works. Data mining theory uses mappings between monoids and semiring structures. Grobner Basis to solve simultaneous multivariable polynomial equations use the theory of Rings and Ideals. Another important abstract structure used in computer science is lattice [8], consisting of a partially ordered set in which every two elements have a unique supremum (also called a least upper bound or join) and a unique infimum (also called a greatest lower bound or meet). The set of natural numbers is an example of lattice, partially ordered by divisibility, for which the unique supremum is the least common multiple and the unique infimum is the greatest common divisor. Lattices can also be characterized as algebraic structures satisfying certain axiomatic identities. Because meet and join both commute and associate, a lattice can be viewed as consisting of two commutative semigroups. Lattice theory was mixed with Topology to develop continuous lattices, which are continuous as posets formed the foundations for Denotational Semantics, which is an approach of formalizing the meanings of programming languages by

constructing mathematical objects (called denotations) that describe the meanings of expressions from the languages.

Conclusion

Mathematics in all its forms is used excessively in numerous branches of science. Only a few applications are discussed here. Apart from these areas, it has applications in Economics, Commerce, Molecular biology, Botany, Zoology, Geology, Information Technology and a lot of other sciences. This may be the reason for considering mathematics as the crest of peacock among sciences in ancient India. A clear knowledge of mathematics makes it easy to understand the principles behind every theory.

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