The Periodic Table: Chemical Properties and Mendeleev Meets Physical Properties and Machine Learning

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Abstract. The periodic table, a fundamental tool in chemistry, has undergone a remarkable evolution from its early qualitative studies to the integration of modern machine learning applications. This paper delves into the historical journey of the periodic table, highlighting key events and contributions from renowned scientists such as Mendeleev, Moseley, and Bohr. Through their groundbreaking work, our understanding of the elements and their periodic trends has been significantly enhanced. The periodic table's predictive power, rooted in the periodic law, has not only facilitated the systematic organization of elements but has also enabled the anticipation of properties of yet-to-be-discovered elements. With the advent of machine learning algorithms, researchers now have the capability to predict the properties of novel elements, optimize experimental conditions, and accelerate the discovery of new materials. This paper explores the enduring significance of the periodic table as a symbol of order and discovery in the field of chemistry, showcasing its continued relevance and utility in the context of modern scientific advancements and technological innovations.

Keywords: Periodic table · Chemistry · Evolution · Mendeleev · Moseley · Bohr · Machine Learning · Periodic Trends · Predictive Modeling · Element Properties

1 Introduction

The periodic table is a fundamental tool in chemistry that organizes the elements based on their properties and atomic structure. The history of the events that have punctuated the development of the modern periodic table as we know it today goes back a long way. In its earliest form, qualitative studies led to the grouping of similar elements like copper, silver and gold. The transition to

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quantitative chemistry was marked by Lavoisier and Richter, laid the foundation for the establishment of laws of chemical combination and the concept of atomic weights introduced by Dalton. The Periodic Table embodies the periodic law and system, serving as a cornerstone of the discipline and inspiring new analogies and relationships within chemistry. The impact of modern physics on the periodic table with the contributions of Quantum Physics stalwarts such as Moseley and Bohr influenced the understanding of atomic structure and the organization of the elements [1].

In the current realm of technological revolution it is undeniable that Machine learning (ML) has revolutionized the field of chemistry by providing powerful tools to analyze complex data, predict outcomes, and accelerate research processes. One of the key contributions of ML to chemistry is in the analysis of large datasets. Chemists have long collected and compiled data on various aspects of chemical properties and reactions. ML algorithms can process this vast amount of data to extract valuable insights, identify patterns, and make predictions. By leveraging ML, researchers can uncover hidden relationships between variables, discover new trends, and optimize experimental conditions. Moreover, ML plays a crucial role in predictive modeling and optimization.

By training ML models on experimental data, researchers can predict the outcomes of chemical reactions, properties of materials, and behavior of molecules with high accuracy. This predictive capability is invaluable in designing new compounds, optimizing reaction conditions, and accelerating the discovery of novel materials. In the realm of chemical informatics, ML algorithms are used to extract chemical structures and reactions from the literature, annotate chemical patents, and improve access to chemical data through platforms like PubChem. These applications streamline the process of data retrieval and analysis, enabling researchers to access a wealth of information quickly and efficiently [2]. The goal of this research is to inform and educate an audience that is not privy to the sophisticated elements that forms the edifice of the two disciplines explored as to how the elements of one can be extrapolated and used to discern pertinent insights from the other.

The paper is organized in the following sequence. In Sect. 2 we outline the properties of the elements in the periodic table and the idiosyncrasies in the patterns of variability along the horizontal and vertical dimensions. In Sect. 3 we outline the existing pedagogy that has contributed to this domain and subsequently analyze a panoply of periodic machine learning algorithms and compare their performances. We also scrutinize the ability of multi-class classification machine learning models to predict the class and period of elements based on their physical and chemical properties. In Sect. 4 we discuss the conceivable pedantic contributions that our research has in the interdisciplinary rubric of Computer Science and Physical Science. In Sect. 5 we summarize the key ideas that form the bedrock of the project and our quantitative findings that are prescient to form coherent paths towards future endeavors. In Sect. 6 we posit the direction that the research will take going forward and the various tangential

methods that we will explore to solve the central questions posed in this research project so as to garner higher values of performance indicators.

2 Literature Survey

2.1 Discovery of Elements

The history of modern chemistry is said to have begun with Robert Boyle's distinction of chemistry from alchemy in 1661. Another crucial advancement was made by Antoine Lavoisier, often referred to as the Father of Modern Chemistry, who developed the law of conservation of mass in 1789. Lavoisier's work was instrumental in establishing chemistry as a full-fledged science. He is credited with recognizing sulfur as an element in 1777 and naming hydrogen (1793), oxygen (1777), and nitrogen (1776). Nicolas-Louis Vauquelin's discovery of beryllium (Be) in beryl and emerald, as well as chromium (Cr) in 1797, further contributed to the expanding knowledge of chemical elements. Additionally, H. Klaproth's observation of uranium in 1789 and E.-M. Péligot's naming of it after the recently discovered planet Uranus demonstrate the interconnectedness of scientific discoveries and astronomical events.

The 18th century was a period of significant change and progress in Europe, marked by events such as the French Revolution (1789–1799) and the emergence of new ideas in science and philosophy. These societal transformations influenced the development of science, leading to breakthroughs in chemistry. The discovery of uranium (U) in France and Germany during this time laid the groundwork for future advancements in nuclear power and atomic research. The discovery of chemical elements is punctuated by fleeting periods of ingenious discovery and intellectual stagnation. This cyclical pattern reflects the ebb and flow of scientific exploration and the influence of external factors on research and discovery. Political and economic changes have played a significant role in shaping the course of scientific investigations, with obstacles sometimes hindering progress but not halting the pursuit of knowledge. In more recent times, the collaboration between the United States and Russia in supplementing the Periodic Table with new elements, such as Flerovium (Fl) and Livermorium (Lv) in 2009 and 2010, exemplifies the global nature of scientific discovery. The dismantling of barriers, like the Berlin Wall, has paved the way for international cooperation in advancing our understanding of the chemical world [3].

Marie Curie's groundbreaking work in the late 19th century involved isolating radioactive elements like polonium and radium from pitchblende ore. By measuring the activities of these elements, she introduced the concept of radioactivity and developed the unit of measurement known as the Curie (Ci). This laid the foundation for quantifying the radioactive decay of substances, leading to the establishment of the Becquerel (Bq) as the standard unit for activity measurement. The periodic table of elements, as envisioned by Dmitri Mendeleev in the 19th century, provided a framework for organizing the known elements based on their atomic weights and chemical properties.

Mendeleev predicted eka-aluminium and eka-tellurium, which later proved to be accurate with the discovery of gallium and polonium, respectively. The narrative then shifts to the 1940s, a period marked by significant advancements in nuclear science. The discovery of trans-uranium elements, including plutonium, thorium, and neptunium, expanded the periodic table beyond uranium. These elements, part of the actinide series, played a crucial role in nuclear research and energy production. The International Year of the Periodic Table in 2019 celebrated the 150th anniversary of Mendeleev's periodic chart, underscoring the enduring significance of this foundational scientific tool. The periodic table now encompasses elements up to Z = 118, reflecting the continuous exploration and discovery of new elements over the years [4]. A brief historical disposition of the elements is given in Table 1.

Table 1. History of Discovery of Elements

Year	Element
Antiquity	Au, Ag, Cu, Fe, Sn, Pb, Sb, Hg, S, C, N
Middle Age	As, Bi, Zn, P
1730	Co, Pt
1750	Ni, Mg
1760	H
1770	N, O, Cl, Mn, Ba
1780	Mo, W, Te, Zr, U, Sr
1790	Ti, Y, Be
1800	V, Nb, Ta, Rh, Pa, Ir, Ce, K, Na, B, Ca, Ru, Ba
1810	I, F, Li, Se, Cd
1820	Si, Al, Br, Th
1830	La
1840	Er, Tb
1860	Cs, Rb, Tl, In, He
1870	Ga, Ho, Yb, Sc, Tm
1880	Gd, Pr, Nd, Ge, Dy, Sm
1890	Ar, Kr, Ne, Xe, Po, Ra, Ac
1900	Rn, Eu, Lu
1910	Pa, Re
1920	Hf
1930	Fr, Tc
1940	Np, At, Pu, Cm, Am, Pm, Bk
1950	Cf, Es, Fm, Md, No
1960	Lr, Rf, Db
1970	Sg
1980	Bh, Mt, Hs
1990	Ds, Rg, Cu
2000	Fl, Lv

2.2 Delineation of Intrinsic Properties of Elements

Periodic properties in the periodic table refer to the trends that repeat at regular intervals as one moves across a row or down a column. These trends are crucial for predicting the behavior of elements and their compounds based on their position in the table. Key periodic properties include valence electron configurations, valence numbers, sizes, and energies of valence shells. These properties exhibit principal and secondary periodicity, highlighting the underlying patterns in element chemistry. There is a pertinent significance of considering the valence electron configurations of bonded atoms in chemical compounds rather than relying solely on the ground states of free atoms. This shift in perspective allows for a more accurate representation of chemical behavior in various conditions.

Additionally, elements with closed and inert valence shells, such as (sp)8, (d)10, and (f)14 configurations, serve as fix-points of chemical periodicity, influencing the reactivity and stability of these elements. Non-periodic properties, on the other hand, encompass unexpected chemical behavior that deviates from traditional periodic trends. These phenomena challenge conventional assumptions and require a nuanced understanding of complex chemical interactions. By combining experimental data with theoretical insights, researchers can uncover hidden patterns and anomalies in element chemistry. One of the key challenges in understanding periodic and non-periodic properties lies in reconciling theoretical models with experimental observations. A multitude of theoretical frameworks found in the seminal works of the pioneers of modern physics provide the understanding of the observed trends in element chemistry and the properties of unknown elements. Certain elements show idiosyncratic complexities such as hydrogen and transition metals due to their variable oxidation states [5].

One of the elements that became a topic of controversy was Hafium (Atomic Number: 72). It was anticipated that element 72 would be classified among the transition metals and would have similarities to zirconium, element 40. This prediction set the stage for the eventual discovery of hafnium by Dirk Coster and Georg von Hevesy, who conducted their research at Niels Bohr's laboratory in Copenhagen. The duo's meticulous search in zirconium minerals led to the identification of hafnium, a discovery that was officially announced in a paper published in January 1923. However, the road to accepting hafnium as a new element was far from smooth. Resistance came from French chemist Georges Urbain, who had previously proposed celtium as element 72. Urbain's refusal to concede, coupled with allegations of credit-stealing and scientific disputes, created a tense atmosphere within the scientific community. The debate extended across borders, with scientists from different countries taking sides based on national affiliations and scientific beliefs [6].

The periodic table is emblematic in addressing a litany of essential questions pertaining to few chosen themes that range from limiting the number of elements, establishing relationships between element properties and composition of substances, that provide a framework for the chemical behavior of elements [7].

2.3 Dmitri Mendeleev and the Watershed Breakthrough

Dmitri Mendeleev's groundbreaking work on the periodic table of chemical elements revolutionized the field of chemistry and laid the foundation for modern understanding of the elements and their properties. In his 1869 paper titled "Relation of the Properties to the Atomic Weights of the Elements," Mendeleev introduced the concept of the periodic law, which stated that the properties of elements are a function of their atomic weights and exhibit periodic trends. This simple yet profound idea transformed the way scientists classified and understood the elements, leading to a systematic organization of the known elements and the prediction of undiscovered ones.

Mendeleev's approach to developing the periodic table was unique in that he used both the atomic weights of elements and their chemical properties to arrange them in a logical order. The columns in the same group exhibited similarity in chemical properties, more specifically the formation of oxides and hydrides (See Fig. 1). By arranging the elements in rows and columns based on their atomic weights and similarities in properties, Mendeleev was able to identify gaps in the table where undiscovered elements should exist (See Fig. 2). This predictive power of the periodic table was one of its most remarkable features, as it allowed Mendeleev to anticipate the properties of elements that had not yet been isolated or characterized.

One of the key aspects of Mendeleev's work was his recognition of the periodicity in the properties of elements. He observed that as one moved across a row in the periodic table, the properties of elements exhibited a regular pattern of variation. This periodicity allowed Mendeleev to group elements with similar properties together and predict the properties of missing elements based on their position in the table. This predictive power was a testament to the underlying order and structure of the elements in nature.

In addition to his work on the periodic table, Mendeleev made significant contributions to other areas of chemistry. He studied the origins of petroleum and proposed the "abiotic origin" hypothesis, suggesting that hydrocarbons originated from iron carbides deep within the Earth. Mendeleev's insights into the origins of petroleum and his work on catalysis laid the groundwork for future research in these areas.

Mendeleev's periodic table not only provided a systematic framework for organizing the elements but also paved the way for further discoveries in chemistry. His periodic law, which highlighted the relationship between atomic weights and properties, represented a fundamental natural system of classification that continues to be a cornerstone of modern chemistry. The periodic table remains one of the most iconic and recognizable symbols in science, representing the building blocks of nature and the intricate relationships between the elements [8].

In Mendeleev's periodic table, elements within the same group or column exhibited similar chemical behavior. For example, elements in Group I (alkali metals) and Group VII (halogens) showed similarities in forming compounds. The alkali metals readily formed oxides and hydrides, while the halogens were

known for their ability to form halides. By observing the trends in the periodic table, Mendeleev could predict the properties of elements that had not yet been discovered. For instance, he predicted the existence and properties of ekaboron (later identified as scandium) based on its expected similarities to boron and aluminum. Mendeleev anticipated that ekaboron would form oxides and hydrides similar to those of boron and aluminum, showcasing the predictive power of his periodic table [9].

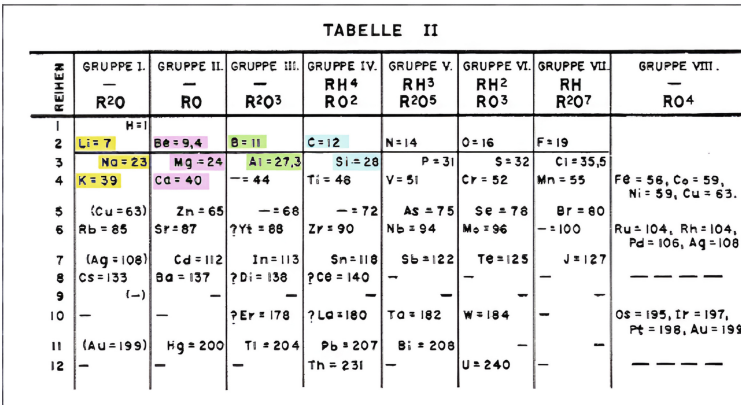

TABELLE II

REIHEN	GRUPPE I. — R^2O	GRUPPE II. — RO	GRUPPE III. — R^2O^3	GRUPPE IV. RH^4 RO^2	GRUPPE V. RH^3 R^2O^5	GRUPPE VI. RH^2 RO^3	GRUPPE VII. RH R^2O^7	GRUPPE VIII. — RO^4
1	H=1							
2	Li = 7	Be = 9,4	B = 11	C = 12	N = 14	O = 16	F = 19	
3	Na = 23	Mg = 24	Al = 27,3	Si = 28	P = 31	S = 32	Cl = 35,5	
4	K = 39	Ca = 40	— = 44	Ti = 48	V = 51	Cr = 52	Mn = 55	Fe = 56, Co = 59, Ni = 59, Cu = 63.
5	(Cu = 63)	Zn = 65	— = 68	— = 72	As = 75	Se = 78	Br = 80	
6	Rb = 85	Sr = 87	?Yt = 88	Zr = 90	Nb = 94	Mo = 96	— = 100	Ru = 104, Rh = 104, Pd = 106, Ag = 108
7	(Ag = 108)	Cd = 112	In = 113	Sn = 118	Sb = 122	Te = 125	J = 127	
8	Cs = 133	Ba = 137	?Di = 138	?Ce = 140	—	—	—	— — — —
9	(—)	—	—	—	—	—	—	
10	—	—	?Er = 178	?La = 180	Ta = 182	W = 184	—	Os = 195, Ir = 197, Pt = 198, Au = 199
11	(Au = 199)	Hg = 200	Tl = 204	Pb = 207	Bi = 208	—	—	
12	—	—	—	Th = 231	—	U = 240	—	— — — —

Fig. 1. Mendeleev's Periodic Table with elements forming similar oxides and hydrides in the same group [9]

2.4 Gaps in Mendeleev's Periodic Table

One of Mendeleev's most significant contributions was his ability to predict the existence and properties of undiscovered elements. He used the concept of "eka" elements, where he named and described hypothetical elements that would fill the gaps in his periodic table [10]. For example,

- Mendeleev predicted an atomic mass of 44 for ekaboron in 1871. The discovered element, scandium, had an atomic mass of 44.955910.
- He predicted the atomic mass of eka-aluminum to be 68, while the actual mass of gallium turned out to be 69.3.
- He predicted the atomic mass of eka-silicon to be 72, and the atomic mass of the discovered element germanium was 72.59.

In more recent times, the discovery of radioactive elements and decay experiments have lead to the discovery of increasingly larger atoms with very high Atomic Numbers which require specialist equipment and techniques to discover. This was made possible by the invention of the cyclotron one of the first particle accelerators invented by Ernest Lawrence in 1920 [11].

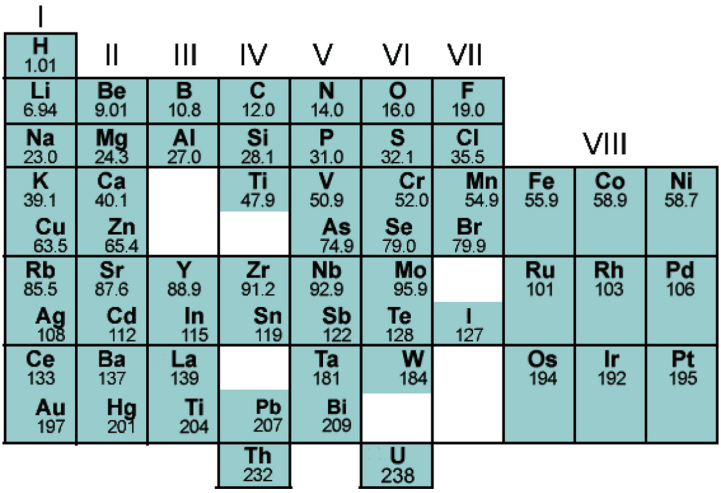

Fig. 2. Gaps in Mendeleev's Periodic Table [10]

2.5 Modern Periodic Table

Since Dmitri Mendeleev, many scientists have made efforts to accommodate the discovery of novel elements in the periodic table and make amendments to the existing table. Henry Moseley's groundbreaking work in X-ray spectroscopy revolutionized the field of chemistry by addressing the limitations of arranging the periodic table by atomic weight. Prior to Moseley's experiments, the periodic table was organized based on atomic weight, a concept that posed several challenges and inconsistencies. Atomic weight, while initially thought to be a fundamental property of elements, presented issues such as anomalies in the ordering of elements and a lack of predictive power in determining element properties. The arrangement of the periodic table by atomic weight led to discrepancies in the positioning of elements, as some elements did not align with their expected properties based on atomic weight alone. This lack of consistency hindered the ability to accurately predict the behavior and characteristics of elements, limiting the understanding of the relationships between different elements.

Additionally, the concept of atomic weight did not provide a systematic way to organize the elements, leading to confusion and inaccuracies in the periodic table. Henry Moseley recognized these limitations and sought to address them through his experiments with X-ray spectroscopy. By studying the frequencies of X-rays emitted by elements when bombarded with cathode rays, Moseley made a groundbreaking discovery - the frequencies of X-rays were characteristic of each element and directly related to the charge on the atomic nucleus of the element. This relationship between X-ray frequencies and atomic number provided a more accurate and reliable way to categorize elements. Moseley's key contribution was the introduction of atomic number as the basis for organizing the periodic table. Instead of relying on atomic weight, Moseley proposed

that elements should be arranged in order of increasing atomic number, which corresponds to the number of protons in the nucleus of an atom. This reorganization by atomic number provided a more logical and predictive framework for understanding the properties and behaviors of elements.

By redefining the periodic table based on atomic number, Moseley's work brought a new level of precision and coherence to the field of chemistry. The modern periodic table is given in Fig. 3. The concept of atomic number allowed for a more systematic arrangement of elements, where elements with similar properties were grouped together based on their atomic structure rather than their atomic weight. This reorganization not only resolved the inconsistencies and anomalies present in the previous arrangement by atomic weight but also laid the foundation for a more comprehensive understanding of the periodic table [12].

Recent studies by researchers like Eric Scerri and Geoff Rayner-Canham have provided valuable insights into the structure and patterns of the periodic table. These studies have challenged traditional views and expanded our understanding of the relationships between elements. For example, Scerri's work has delved into the complexities of the periodic table, revealing that the relationships between elements are more intricate than initially perceived. This nuanced approach has opened up new avenues for exploration and understanding in the field of chemistry. Furthermore, Gärditz discusses the importance of acknowledging and learning from errors in scientific discourse. He argues that the process of scientific cognition involves methodically disciplined errors that are essential for progress. By embracing the imperfections and uncertainties inherent in scientific research, we can foster a more robust and dynamic scientific community. The review also touches upon the evolving nature of scientific knowledge and the need for interdisciplinary collaboration. Gärditz highlights the interconnectedness of different fields of study and the importance of transcending language and system boundaries to advance scientific understanding. This holistic approach underscores the significance of long-term perspectives and collaborative efforts in driving scientific progress [13].

The Pauli Exclusion Principle has found an imperative significance in the modern periodic table. Pauli's Exclusion Principle states that no two electrons in the same atom can have identical values for all four of their quantum numbers. The orbitals in an orbit are described using the principal quantum number (n) and azimuthal quantum number (l). There are $2l + 1$ distinct orbitals for each set of n and l. Each shell is subdivided into multiple subshells (s, p, d, f). Number of electrons in each shell increases with the atomic number and successive electrons go into less stable shells. The numbers 2, 8, 18, 32 correspond to s; s and p; s, p, and d; s, p, d, and f subshells, respectively [14].

2.6 Machine Learning: A Few Common Facts

Machine learning (ML) is a branch of artificial intelligence (AI) that focuses on developing algorithms and models that enable computers to learn from data and make predictions or decisions without being explicitly programmed. ML

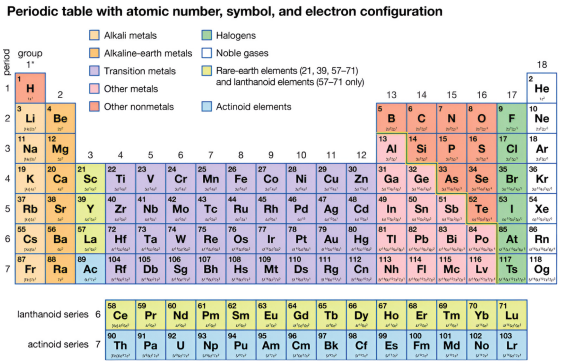

Fig. 3. Modern Periodic Table of Mosley [13]

algorithms use statistical techniques to identify patterns in data, learn from these patterns, and make informed decisions or predictions based on new data. This process allows machines to improve their performance over time as they are exposed to more data. One of the key concepts in machine learning is the use of datasets, which are collections of data points or samples that represent entities to be analyzed. Each data point consists of features, which are specific properties or characteristics of the entity being studied. For example, in a medical context, a dataset could consist of patient data, with features such as age, gender, and medical history. These features are used by ML algorithms to make predictions or classifications based on patterns in the data.

There are two main types of machine learning: supervised learning and unsupervised learning. Below is an explanation of each type:

1. **Supervised Learning**: In this type of learning, the algorithm is trained on labeled data, where the correct output is provided for each input. The algorithm learns to map inputs to outputs, enabling it to make predictions on new, unseen data. Supervised learning tasks include:
   (a) **Regression**: The goal is to predict a continuous value.
   (b) **Classification**: The goal is to assign inputs to predefined categories.
2. **Unsupervised Learning**: In unsupervised learning, algorithms are trained on unlabeled data, where the goal is to discover patterns or structures within the data. Unsupervised learning tasks include:
   (a) **Clustering**: The algorithm groups similar data points together.
   (b) **Dimensionality Reduction**: The algorithm reduces the number of features while preserving important information.

Machine learning models can range from simple and interpretable, such as linear regression or decision trees, to complex and less interpretable, such as deep neural networks. The choice of model depends on factors such as the complexity of the data, the desired level of interpretability, and the performance requirements of the task at hand. The field of machine learning has seen significant

advancements in recent years, driven by the availability of large datasets, powerful computational resources, and improved algorithms. These advancements have led to breakthroughs in various scientific domains, including biology, medicine, and pharmacology. Machine learning techniques are being used to analyze complex biological data, such as genetic sequences and medical images, to uncover patterns and insights that can inform drug discovery, disease diagnosis, and treatment optimization [15].

2.7 Machine Learning for Periodic Systems

One of the indispensable features of a periodic table is the repetitive similarity in properties observed in quantitative intervals. To delineate this periodicity through machine learning one has to use a framework with an underlying periodic function that best fits the data. Several such dispositions have been explored where machine learning has been used to the explain the inherent pattern in various sets of data from an eclectic array of domains. One of the approach involves combining machine learning (ML) techniques with the Density Functional Tight Binding (DFTB) method to enhance the accuracy and efficiency of electronic structure calculations for periodic systems with defects [16].

In the article "Adapting Machine Learning Technique for Periodicity Detection in Nucleosomal Locations in Sequences" the authors delve into the innovative use of a dynamic periodicity detection algorithm to uncover patterns in DNA sequences related to nucleosome positioning [17]. The article "Representing Periodic Functions with Boundaries and Enforcing Exact Periodic Conditions with Deep Neural Networks" by Suchuan Dong and Naxian Ni from Purdue University introduces a novel method that leverages deep neural networks (DNNs) to represent periodic functions and enforce exact periodic boundary conditions. The traditional numerical methods for solving differential equations are being challenged by the emergence of DNNs, which transform the problem into an optimization task and represent the unknown field function using the universal approximation property of neural networks [18].

The article "Deep Learning View of Periodicity" explores the application of deep learning in understanding and forecasting periodic time series data. It introduces a novel framework called DEPTS (Deep Expansion Learning for Periodic Time Series Forecasting) to address the challenges associated with modeling complicated dependencies and diverse periods in periodic time series. DEPTS leverages deep neural networks to progressively expand the understanding of the dependencies of periodic time series signals on periodicity. The framework introduces a decoupled formulation for periodic time series forecasting by incorporating a hidden periodic state variable. This approach allows for customized designs to handle the specific challenges posed by periodic time series data [19].

3 Periodic Table Using Machine Learning

There has been scanty research on the utilitarian aspects of machine learning to create the modern periodic table using the properties of elements as features. The

article "Recreation of the periodic table with an unsupervised machine learning algorithm" explores the application of unsupervised machine learning to recreate the periodic table based on observed physicochemical properties of elements. The study introduces the Periodic Table Generator (PTG), an innovative algorithm that automates the translation of high-dimensional data into a tabular form with varying layouts to capture the underlying periodicity and similarity of elements. The PTG leverages Generative Topographic Mapping with Latent Variable Dependent Length-Scale and Variance (GTM-LDLV) to represent complex response surfaces of elemental data in a lower-dimensional space. By mapping chemical elements onto regular grid points in a latent space, the PTG organizes the elements into a two-dimensional array resembling Mendeleev's periodic table or a three-dimensional spiral table. This process involves compressing element features, such as melting point and electronegativity, into reduced-dimensional latent spaces to capture the essence of the elements' physicochemical properties [20].

CNNs have demonstrated remarkable success in image recognition tasks due to their ability to extract meaningful features from complex data. In a study, the researchers aimed to harness the power of CNNs to learn the inner structure and chemical information embedded in the periodic table. By representing the periodic table as a matrix and initializing it with specific values, the CNN was trained to understand the relationships between elements and their properties. The PTR approach involved setting specific values in the matrix corresponding to element positions to facilitate learning. By manipulating the matrix values and multiplying it by 20 to mimic a digital image, the researchers aimed to ease the training process of the CNN. This innovative representation allowed the CNN to capture the two-dimensional layout of the periodic table and extract relevant chemical information [21].

In our research, we focused on two specific fronts of this milieu. Firstly, we analyze the presence of periodicity in the chemical and physical properties with change in atomic weight and atomic number in a scrupulous attempt to find the best periodic function that can fit the variation in chemical and physical properties. Secondly, we try to use multi classifiers to predict the position of elements in the modern periodic table by using group number and period number as the dependent variables and the chemical and physical properties as the independent variable.

3.1 Predicting Periodicity in Physical Properties: Melting and Boiling Points

The melting point and boiling point of elements are physical properties linked to the type of structure that the element exists in. The general trend in the period table across a group shows an increase in melting and boiling points from group 1 to group 4 after which it plummets slowly till group 8. The underlying reason for this behavior is the fact that in group 1 to 4, the elements exist in giant structures, and from group 5 to group 8 they exist as molecules. Jan-Michael Mewes

and Peter Schwerdtfeger in their seminal article "Exclusively Relativistic: Periodic Trends in the Melting and Boiling Points of Group 12" explore the domain of quantum chemistry by focusing on the melting and boiling points of Group 12 elements - Zn, Cd, Hg, and Cn. The researchers observed a unique trend in the melting and boiling points, which was predominantly driven by relativistic effects. At a non-relativistic level, the melting and boiling points of Group 12 elements were surprisingly similar, indicating that periodic trends in this group are primarily influenced by relativistic effects. This highlights the significance of considering relativistic effects in understanding the behavior of heavy elements. The article also discusses the empirical relation between phase-transition temperatures and cohesive energies, highlighting the strong correlation between these properties. By analyzing the cohesive energies of Group 12 elements, the researchers were able to estimate the impact of relativistic effects on the transition temperatures, providing valuable insights into the underlying mechanisms driving these changes [22]. In our project we used a kaggle dataset that delineates the information of physical and chemical properties of elements that are part of the periodic table along with their position in the modern periodic table. The details of the elements and their physical properties are mentioned in Table 2. Mendeleev's assertion of the dependence of periodicity on atomic weight was amended due to a few exceptions and the periodicity was later seen depending on atomic number more accurately. We visualized how the melting and boiling point changes with increase in atomic number and atomic weight. The variation in physical properties (melting and boiling points) with atomic number and atomic weights is given in Figs. 4 and 5. As we can see, the peaks and valleys in the graphs illustrates the presence of periodicity with the atomic number showing more consistency as the change is consecutive unlike the atomic weight where the possible value of atomic weight can be either '2n' or '2n + 1' where'n' is the atomic number.

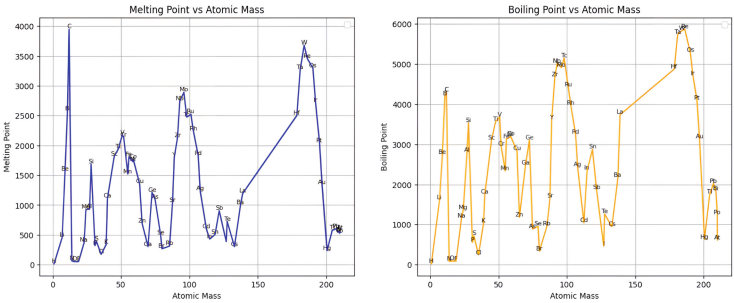

Fig. 4. Change in Melting and Boiling Point with atomic weight

In our analysis, the primary features used are atomic mass and atomic number while the targets are boiling points and melting points. The data is divided into training and testing sets to allow for model training and validation. If

Table 2. Periodic Table of Elements

#	Weight	Element	Symbol	Period	Group	Melting	Boiling
1	1.007	Hydrogen	H	1	1	14.175	20.28
3	6.941	Lithium	Li	2	1	453.85	1615
4	9.012	Beryllium	Be	2	2	1560.15	2742
5	10.811	Boron	B	2	13	2573.15	4200
6	12.011	Carbon	C	2	14	3948.15	4300
7	14.007	Nitrogen	N	2	15	63.29	77.36
8	15.999	Oxygen	O	2	16	50.5	90.2
9	18.998	Fluorine	F	2	17	53.63	85.03
11	22.99	Sodium	Na	3	1	371.15	1156
12	24.305	Magnesium	Mg	3	2	923.15	1363
...	...	...	...	...	...	...	...
79	196.967	Gold	Au	6	11	1337.73	3129
80	200.59	Mercury	Hg	6	12	234.43	630
81	204.383	Thallium	Tl	6	13	577.15	1746
82	207.2	Lead	Pb	6	14	600.75	2022
83	208.98	Bismuth	Bi	6	15	544.67	1837
84	210	Polonium	Po	6	16	527.15	1235
85	210	Astatine	At	6	17	575.15	610

we observe the melting and boiling point there is a non-linear repetitive pattern which tradition regression algorithms will not be able to capture. Therefore, to discern this non-linear trend we use periodic machine learning algorithms such as Harmonic Regression, Periodic Kernel, and Random Forest Regression to analyze which out of these algorithms is best able to capture the periodicity in chemical properties of the elements. These ML Regressors offer a flexible framework for modeling relationships in data without imposing strict assumptions on the underlying function form. This flexibility allows these models to capture complex patterns and make accurate predictions in various domains. By defining a distribution over possible functions that fit a set of data points, the algorithms leverage prior knowledge about the nature of functions through the use of kernel functions [23]. We use Mean Absolute Error (MAE) to evaluate these algorithms and the results are presented in Tables 3 and 4 (Figs. 6 and 7).

When predictions are made against atomic weight, the Periodic Kernel Regression (GPR) model demonstrates the lowest MAE values for both boiling and melting points compared to the other models. Specifically, for boiling points, the MAE values are 1333.00 for GPR, 1502.08 for Harmonic Regression, and 1738.08 for Random Forest Regression. Similarly, for melting points, the MAE values are 866.81 for GPR, 809.84 for Harmonic Regression, and 895.04 for Random Forest Regression. This indicates that the GPR model provides more

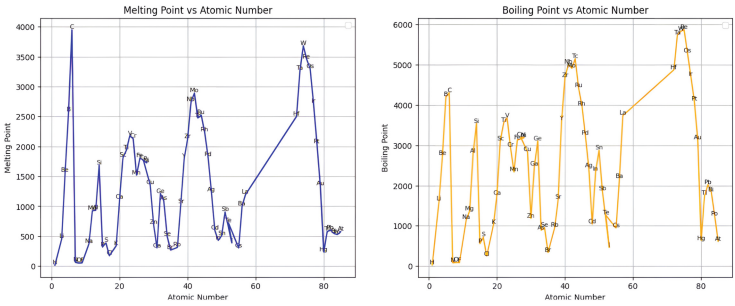

Fig. 5. Change in Melting and Boiling Point with atomic number

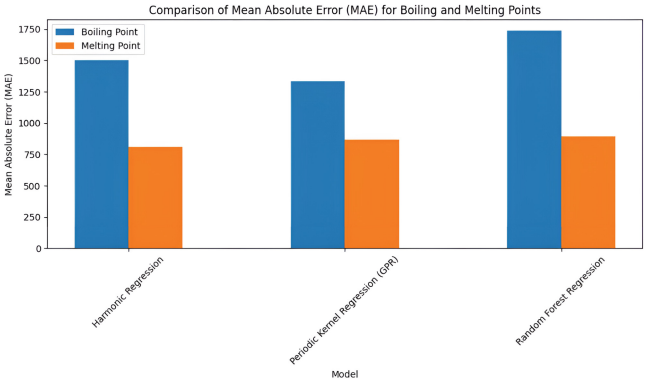

Fig. 6. Comparison Between Various Periodic Machine Learning Algorithm with atomic weight as independent variable

Table 3. Mean Absolute Error (MAE) Values for Boiling and Melting Points against Atomic Weight

Model	Boiling Point MAE	Melting Point MAE
Harmonic Regression	1502.08	809.84
Periodic Kernel Regression (GPR)	1333.00	866.81
Random Forest Regression	1738.08	895.04

Table 4. Mean Absolute Error (MAE) Values for Boiling and Melting Points against Atomic Number

Model	Boiling Point MAE	Melting Point MAE
Harmonic Regression	1562.40	1005.39
Periodic Kernel Regression (GPR)	1426.94	910.17
Random Forest Regression	2207.22	1427.37

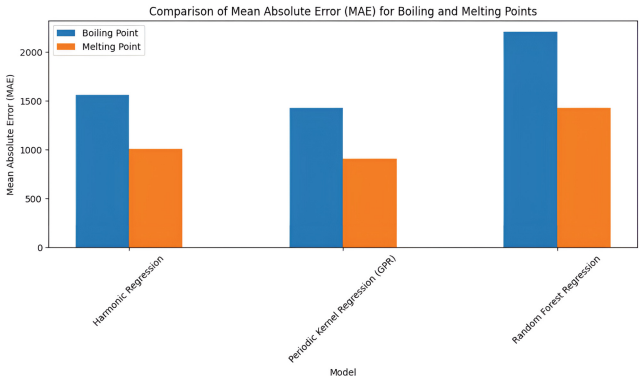

Fig. 7. Comparison Between Various Periodic Machine Learning Algorithm with atomic number as independent variable

accurate predictions for both boiling and melting points when considering atomic weight.

When predictions are based on atomic number, a similar trend emerges. Again, the Periodic Kernel Regression (GPR) model exhibits the lowest MAE values for both boiling and melting points. The MAE values for boiling points are 1426.94 for GPR, 1562.40 for Harmonic Regression, and 2207.22 for Random Forest Regression. Similarly, for melting points, the MAE values are 910.17 for GPR, 1005.39 for Harmonic Regression, and 1427.37 for Random Forest Regression. Thus, regardless of whether predictions are based on atomic weight or atomic number, the GPR model consistently provides the most accurate estimations for both boiling and melting points.

Moreover, a notable observation is that predictions based on atomic weight generally yield lower MAE values compared to those based on atomic number across all models. This suggests that atomic weight may be a more reliable predictor of boiling and melting points than atomic number when using these regression models. This observation is counter intuitive to what we see in the modern periodic table and in many ways vindicates Mendeleev's proposition, therefore a further analysis needs to be done by using more non-linear regression algorithms to discern if the trend remains consistent.

3.2 Reconstructing the Periodic Table Using Machine Learning and Physical Properties

In the context of the periodic table, a period refers to a horizontal row of elements where properties gradually change as you move from left to right. This change is influenced by factors such as atomic weight, ionization potentials, and electron affinity values. The article highlights how the atomic weight plays a significant role in the arrangement, with heavier elements typically positioned lower in the table.

Additionally, irregularities in ionization potentials and electron affinity values across periods are attributed to the effects of filled s shells and half-filled p subshells. On the other hand, a group in the periodic table represents a vertical column of elements that share similar chemical properties. The study demonstrates how elements within the same group exhibit comparable characteristics due to their shared electron configurations. By connecting elements within groups and periods, the periodic table arrangement visually illustrates the periodic trends and relationships among elements based on their atomic properties [24]. In this case study, we used machine learning models to predict the groups and periods of the elements using machine learning models. The results are mentioned below (Table 5):

Table 5. Accuracy of Models for groups and periods

Model	Group Accuracy	Period Accuracy
Random Forest	0.071429	0.285714
SVM	0.285714	0.357143
k-NN	0.071429	0.214286
Naive Bayes	0.357143	0.500000

Naive Bayes performed best overall, achieving 35.7% accuracy for groups and 50% for periods. Gradient Boosting had notable success in predicting periods with 64.3% accuracy. Overall, none of the algorithms provide a very high accuracy in predicting the groups and periods of the elements.

4 Pedagogical Implications

Understanding applications of machine learning to the periodic table of elements offers numerous advantages for science and computer science education. Key pedagogical implications include enhanced comprehension of trends in the analysis of complex chemical and physical phenomena, implementation of interactive tools and visualizations to dynamically illustrate elemental relationships, and use of predictive modeling of new compounds, properties, and behaviors. These types of examples provide educational insights into the pursuit of the scientific method, hypothesis testing, and the process of discovery. Additionally, learners can engage more deeply with cross-disciplinary potential, as integrating machine learning applications with the periodic table highlights connections between chemistry and computer science. An interdisciplinary approach can broaden perspectives and encourage collaboration across fields. Moreover, studying machine learning applications in chemistry encourages students to develop critical thinking skills and proficiency in data analysis. In summary, leveraging machine learning in the context of the periodic table offers exciting opportunities to enhance both science and computer science education. It can transform how students engage

with elemental data, promote active learning, and cultivate skills essential for modern scientific inquiry.

5 Conclusion

The journey of the periodic table from its early qualitative studies to the modern era of machine learning applications has been a testament to the collaborative efforts of scientists across generations. Through the groundbreaking work of figures like Mendeleev, Moseley, and Bohr, we have gained a deeper understanding of the elements and their properties. The contributions of scientists who have been involved in the journey of the formation of the periodic table from Döbereiner to Mendeleev to Mosley forms the overarching umbrella of knowledge having colossal utility in educating seekers who want to garner a deep understanding of the properties of elements. Integrating machine learning in the domain of chemistry has resulted in the formation of a innovative paradigm that intertwines the mathematical tools of data science and the properties of elements contributing to the pedantic literature that already exists on these domains. The periodic table continues to serve as a fundamental tool in chemistry, organizing the building blocks of matter based on their atomic structure and properties. With the integration of machine learning algorithms, researchers are now able to predict the properties of novel elements and accelerate the discovery of new materials. As we look towards the future, the periodic table remains a symbol of order and discovery in the ever-evolving field of chemistry.

6 Future Work

In this research endeavor, we have used supervised machine learning techniques to classify the elements into their respective groups and periods using their chemical properties. The question thus formed, in the parlance of machine learning is a multi-class classification problem. We used three models that use algorithms that can accurately capture the non-linear dependence of chemical properties on boiling points thereby substantiating the presence of periodicity in the variation in properties of the periodic table. The performances of the models were lackluster as they did not provide high accuracy while predicting groups and periods. Therefore, in the subsequent iterations, we will be using unsupervised machine learning algorithms such as hierarchical clustering to group elements with similar chemical properties together. We would also implement neural networks to surmise whether deep learning performs better in discerning periodicity from a supervised learning point of view.

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