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(all content refers to the German school system)

Teaching Structure-Property Relationships with Machine Learning

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Abstract

This article presents a didactic concept that enables the use of a basic machine learning algorithm to work out structure-property relationships in chemistry lessons. The focus is on investigating the boiling points of 1-alkanols and short-chain, branched, monovalent alkanols. With the help of manually supported data organization, students analyze how molecular structural features influence the boiling point. The algorithm used is didactically reduced and mathematically simplified in such a way that it is comprehensible even without programming knowledge at the upper secondary level. In addition, the method introduces the basic principles of machine learning without being tied to a specific programming language. The teaching project presented here was conducted in the first year of upper secondary education. It shows how current developments in digital education and AI can be integrated into chemistry lessons in a didactically meaningful way to promote analytical thinking, the handling of data, and a deeper understanding of chemical relationships.

Keywords: Physical Chemistry – Artificial Intelligence – Computational Thinking

1. Introduction

As noted in a special issue of the journal *Unterricht Chemie* on structure-property relationships, this concept is, from a didactic perspective, a "well-worn hat." [1] Meanwhile, it is counted among the four fundamental basic concepts of chemistry education [2]. However, it requires adaptation to current conditions as well as future developments, such as digitalization. This includes the application of methods of machine learning (ML) to chemical content in order to gain chemical insights. ML has been part of students' everyday lives not only since the introduction of ChatGPT. This fact can also be harnessed for chemistry education.

Talanquer [3] describes six developmental stages in students' understanding of structure-property relationships over the course of their education, which, however, merge into each other fluidly. The focus here is on the final stage, "structural interactionism." The preceding stage, "functional compositionism," i.e., the relationship between the presence of a functional group and substance properties, was dealt with previously in class and is eliminated here by restricting to monovalent alkanols. One of Talanquer's conclusions is that students can benefit from continuous activities involving data analysis, pattern recognition, and model application for understanding structure-property relationships. These are precisely the kinds of activities enabled by using ML.

Parchmann et al. [1] also describe a gradual introduction with increasingly abstract explanations. Similarly, Herzog et al. [4] divide the teaching of structure-property relationships into three levels: (1) recognition and consideration of macroscopic properties and structures,

(2) examination of simple structural models for interpreting properties, and (3) consideration of complex, differentiated models for interpreting and generating structure-property relationships. The teaching sequence here can also be mapped onto this classification.

The teaching topic inherently involves mathematization in chemistry lessons. This is meaningful since theoretical methods of modeling and simulation are established components of chemical research and development. More specifically, group contribution methods [5] represent professional structure-property relationships indispensable in process design in chemical engineering. Quantitative Structure-Property Relationships (QSPR) also correlate molecular properties with macroscopic properties or with biological activity (QSAR). Consequently, the topic of modeling is also included in the KMK educational standards [2], which specify, among others: S10 using chemical concepts to connect issues across disciplines, S17 applying mathematical methods to chemical contexts, and E6 using digital tools for data collection, modeling, and simulation.

Because contributions from mathematics and computer science are also required, the corresponding prerequisites must be considered. These include knowledge of linear functions and the meaning of their parameters (intercept and slope). Prior knowledge of linear regression, however, is not required. The ML regression algorithms are mathematically much simpler than classical regression methods, making regression accessible in chemistry classes in the first place. Programming knowledge is also not required. To develop the regression algorithm, the supporting information (SI) provides a compact manual method as an entry point to the learning algorithm, similar to a method for classification [6].

Here, the boiling points of 1-alkanols and branched monovalent alkanols with up to five carbon atoms are investigated. In addition, the boiling points of other alkanols are predicted. The choice fell on alkanols because, unlike n-alkanes, 1-alkanols exhibit an almost linear relationship between the number of carbon atoms and the boiling point. Moreover, the boiling points of individual alkanols can be determined experimentally in class. After conducting experiments on the boiling points of selected alkanols, a simple model for 1-alkanols and a more complex model involving a structure index were developed. In doing so, both the fundamentals of ML and their application to structure-property analysis are addressed.

2. Machine Learning in Schools

Students are already familiar with ML applications such as translation tools, spellcheckers, and chat programs. However, they usually do not know how such programs work. Understanding the functionality of ML is a prerequisite for assessing its capabilities: What can such a program achieve, and is it intelligent in a human sense? To address such questions, students should first grasp the fundamentals of how ML programs function. A review article [7] analyzed studies on how ML should be taught in schools and concluded that programming with Scratch or Python should be used to demystify ML's core principles. So far, however, there are only a few examples of ML being applied to chemistry topics in secondary education, accompanied by teaching the fundamentals of ML [8-10].

The core of ML can be illustrated by the basic unit of neural networks: the model of a single neuron, such as the Adaline model (adaptive linear neuron) [11]. This is a fundamental model that demonstrates ML principles and is thus not subject to the rapid pace of developments in computer science. Figure 1 shows a scheme for the data flow of a mathematical neuron. The input variables x and y (here, submicroscopic chemical properties) are each multiplied by a weight w_1 and w_2 added together with a constant b corresponding to the intercept. The activation $h(M)$ function then calculates the output z, which here corresponds to a macroscopic property. For the Adaline model, the activation function is linear $h(M) = M$. The learning algorithm, i.e., the optimization of weights, is shown in Figure 2. The error e between the regression line and the experimental data is subtracted from the

parameters. A learning parameter L improves convergence. Details of the algorithm and its classroom implementation, worksheets, and student reactions are provided in the SI.

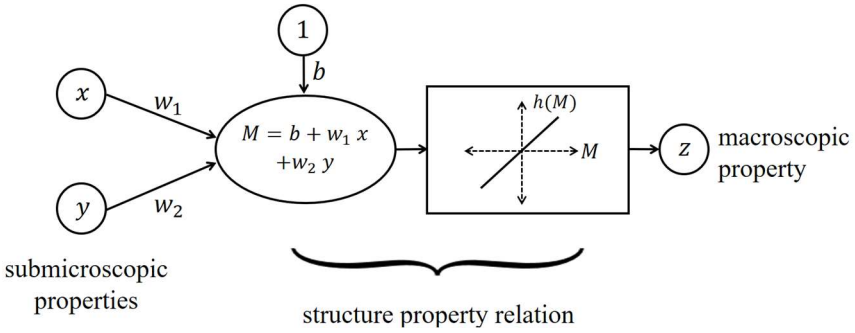


Figure 1: Diagram showing the forward calculation of a three-dimensional regression $z = f(x,y)$ using the Adaline model.

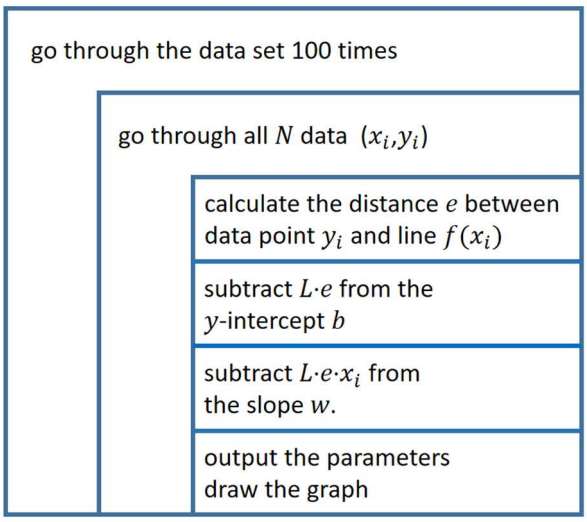


Figure 2: Pseudocode in the form of a Nassi-Shneiderman diagram for the ML algorithm for the regression of a straight line $y = wx + b$. The correction of the parameters is embedded in two loops that run over all N data points and over a certain number of epochs (here 100).

3. Structure-Property Relationships

The number of carbon atoms is used to characterize the substances instead of their mass, as mass has no causal relationship with boiling temperature. When searching the internet, students find sources that argue that molecules with a higher mass require more thermal energy to transition from a liquid to a gaseous state. A list of such sources can be found in the SI. It should be noted that when measuring the boiling point, a system in thermodynamic equilibrium is considered, in which kinetic effects and thus also mass play no role. Only the potential energy based on molecular interactions is included in the phase equilibrium. For example, molecular Monte Carlo simulations of phase equilibrium do not require the molecular mass. The mass of the molecules and that of the carrier gases is only significant in the time-dependent development of a phase transition [12].

3.1 Experiments

Students first determined the boiling point of one alkanol per group. The selected alkanols listed in Table 1 were chosen so that they boil in a water bath and have similar boiling points despite different number carbon atoms. To estimate measurement uncertainty, two groups worked with ethanol. About 20 ml of each alkanol were boiled under reflux in a 100 ml flask in a water bath (Figure 3a). A temperature-time curve was recorded. The boiling point was determined once the temperature remained constant for at least 5 minutes (Figure 3b). The two ethanol measurements differed by 3°C. All values were about 2°C lower than literature values, but the sequence was correct. For example, 2-propanol and 2-methyl-propan-2-ol showed nearly identical boiling points about 4°C higher than ethanol. Beyond yielding boiling points, the experiment also offered an opportunity to discuss phase equilibrium as a dynamic equilibrium on the molecular level.

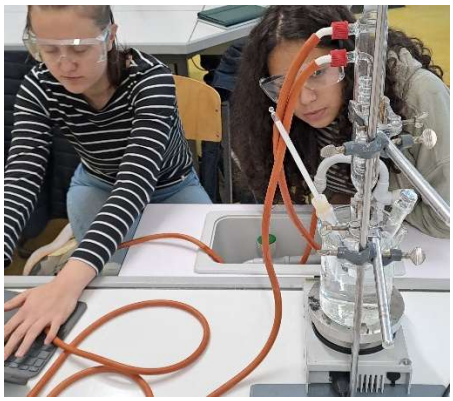
In their first evaluation, the students noted that the boiling points of all investigated alkanols were about 20°C below the boiling point of water. Ethanol had the lowest boiling point, which they attributed to it being the smallest molecule. 2-propanol and 2-methyl-propan-2-

ol had similar boiling points which was related by the students to the a main chain of the same length.

This discussion already revealed the students' suspicion that macroscopic properties are related to molecular properties. On the one hand, they assumed that molecular "size" influences boiling point; on the other, the influence of structure remained unclear.

Alkanol	number of C atoms	b.p. /°C literature [13]	b.p. /°C experiment
Ethanol	2	78,35	75; 78 $\quad \emptyset = 76{,}5$
2-propanol	3	82,24	80
2-methyl-propan-2-ol	4	82,34	80

Table 1: Measured boiling points compared to the literature data.

a) 

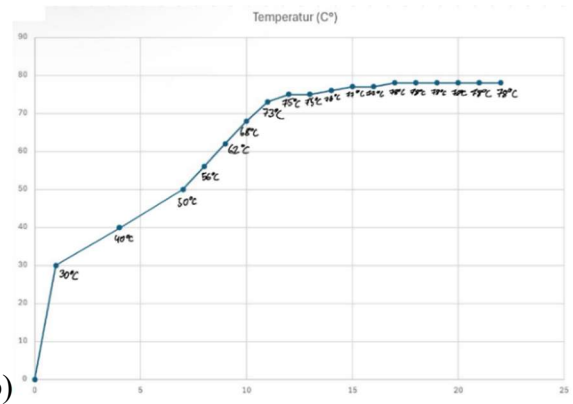
b) 

Figure 3: a) Experiment to measure the boiling temperature of alkanols: A thermometer with a plug is positioned in the gas phase directly above the liquid surface. Strong reflux cooling establishes a boiling equilibrium. b) Plot of temperature as a function of time.

3.2 Regression for 1-Alkanols

After the experimental impulse and the subsequent discussion among the students about the factors influencing the boiling point, the problem was broken down and initially only the unbranched 1-alkanols were considered. To this end, the students looked up the boiling points of the 1-alkanols up to 1-decanol. They recognized that the boiling point increases uniformly with the number of carbon atoms. The number of carbon atoms is an intuitive model that reflects the strength of molecular interaction and is fundamental for further consideration of the influence of structure on the boiling temperature. To test the relationship, a linear regression was performed (for code see SI).

This intermediate step also served to address the principle in a two-dimensional coordinate system in order to be able to move on to the three-dimensional system in the following. In calculus in mathematics lessons, functions with a dependent variable of the type $f(x)$ are addressed. Functions with two dependent variables of the type $f(x, y)$ do not usually appear. At this point, the students were not yet familiar with planes in analytical geometry. For this reason, it makes sense to first perform the regression in the two-dimensional system. Regardless of this, it also makes sense from a chemical point of view to examine the influences on the boiling temperature step by step.

After introducing the ML algorithm (SI), the corresponding program (SI) was made available

so that the students could run it on their iPads. It was also launched on the electronic white-board. The program's animation mode allowed the students to observe the process of parameter iteration, which was analogous to the haptic ML algorithm (SI). By comparing it with the final regression line, the students recognized the slight S-shape of the data (Figure 4). This showed that the line is only a model that is not perfect, but still reflects the course quite well.

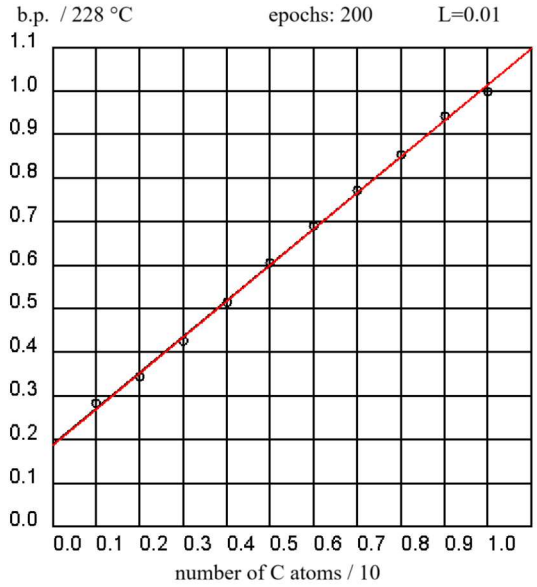


Figure 4: Regression of the boiling temperatures of 1-alkanols as a function of the number of carbon atoms, divided by the corresponding maximum values. The symbols represent experimental data [13]

3.3 Development of a Structure index for Alkanols

An important step in data science is data preparation and organization, which requires expertise in the data. The properties of the objects must be expressed by numbers. Isomers require a number for the degree of branching of the molecules. To develop this, the students were given a worksheet showing the structures of the first 16 alkanols up to C5 (SI). Their task was to find key figures for the structure of the alkanols. As a first key figure, the students spontaneously suggested the length of the longest chain. This consideration resulted from the inclusion of experiments in which the main chains of 2-propanol and 2-methyl-propan-2-ol, which are of equal length, were held responsible for their very similar boiling temperatures. However, since this approach led to the same key figures for different molecules, the students added branching. Since there are not only branched and unbranched molecules, but also single and multiple branches, the students suggested the number of branches as an additional key figure. The students then labeled the 16 alkanols with these codes (Figure 5). It turned out that there are still different molecules with the same code, which are highlighted in the same color in Figure 5. For example, there are three isomers with the longest chain (l.c.) of four C atoms and one branch (br.). To further differentiate them, the students suggested adding the position (pos.) of the branch. This resulted in identical identification numbers only for 2-butanol and 3-pentanol.

Finally, the students were given the task of developing a single structure index from a combination of the key figures that should be as clear as possible. One suggestion from the students was to add and subtract the key figures. However, it quickly became clear that many molecules would then have the same structure index. Another suggestion from the students was to use the key figures as digits of a number, e.g., 411 (l.c.=4, br.=1, pos.=1) for 2-pentanol. For 3-methyl-butane-2-ol, there are branches at two different positions. This was taken into account here by adding a decimal place; one branch at position 1 and one at position 2, resulting in 321.2. A list of these indices is given in the SI. The development of this index was worked out by the students in the discussion without help.

Developing a structure index comparable to one used in specialist science would certainly not be possible for students. The discussion in the course is therefore an analog discussion in which the students work through the ideas necessary for development. One might initially assume (see, however, section 3.5) that the result is not optimal. However, the students understood the idea of a structure index as a measure. In addition, in the course of this discussion, the students dealt intensively with the nomenclature, the framework structures, and the possible isomers, so that they were able to handle them confidently afterwards.

Structure indices are based on a paper by Randic [14], which served as the basis for the

development of a large number of so-called connectivity indices in the literature. For further discussion of the topic in class, a structure index was chosen that is mathematically much simpler than the indices found in the technical literature. To do this, the lengths of the C chains from the O atom to the ends of the strands of a molecule are determined, as shown in the upper section in Figure 6. These lengths of no more than three chains are designated a, b, and c. For the structure index I, the reciprocal values of these chain lengths are added:

$$I = \frac{1}{a} + \frac{1}{b} + \frac{1}{c} \qquad (1)$$

If a variable is equal to zero, the corresponding term in the above equation is omitted. This is a simple structural model in which the index increases differentially with increasing branching. It is therefore suitable for correlating a higher degree of branching with weaker interaction.

3.4 Manual regression

The students were given 16 cards with alkanols containing up to five carbon atoms. These cards (Figure 6) contain the name, the skeleton structure, the boiling point, the number of carbon atoms, and the structure index I. The students were given the task of sorting the cards in order to identify a systematic pattern. No sorting criterion was specified in order to allow for different hypotheses. Each group tried out several possibilities. Some groups initially placed the cards in a row with increasing boiling temperature, others with increasing structure index. One group sorted the cards directly in two dimensions according to the number of carbon atoms and the structure index. In doing so, they recognized that the boiling temperature decreases systematically from one corner of their sorted cards to the opposite corner. The other groups tried out several possibilities and finally also arrived at a two-dimensional sorting. Figure 6 shows the final sorting of the cards (see also SI). The students were asked to hold a plane above the sorted cards whose height corresponded qualitatively to the boiling temperature. This haptic representation of the regression plane was intended to facilitate understanding of the subsequent digital regression and its representtation on the screen. In addition, one group noticed that the sequence of boiling temperatures of 2-pentanol and 3-pentanol (circled in red in Figure 6) deviates from the series. This shows once again that a structure index is not perfect.

3.5 Boiling Points of Branched Alkanols

In the second step, three-dimensional ML regression was performed as a function of the carbon number and the structure index I using the computer program (SI) (Figure 7a). The regression plane moves toward the points. It was found that the linear regression model is not exact, as some points lie below it and others above it. Overall, however, the boiling temperatures can be well described by the plane. In individual discussions, all groups explained, based on the graph, that the dependence on the number of carbon atoms is greater than that on the structure index. They recognized this from the slopes in the graph in both directions. The signs of the slopes also made it clear that the boiling temperature rises with increasing carbon number and decreases with increasing branching. The students had to establish a direct connection between mathematical and chemical content, i.e., the findings resulted from the combination of both subjects.

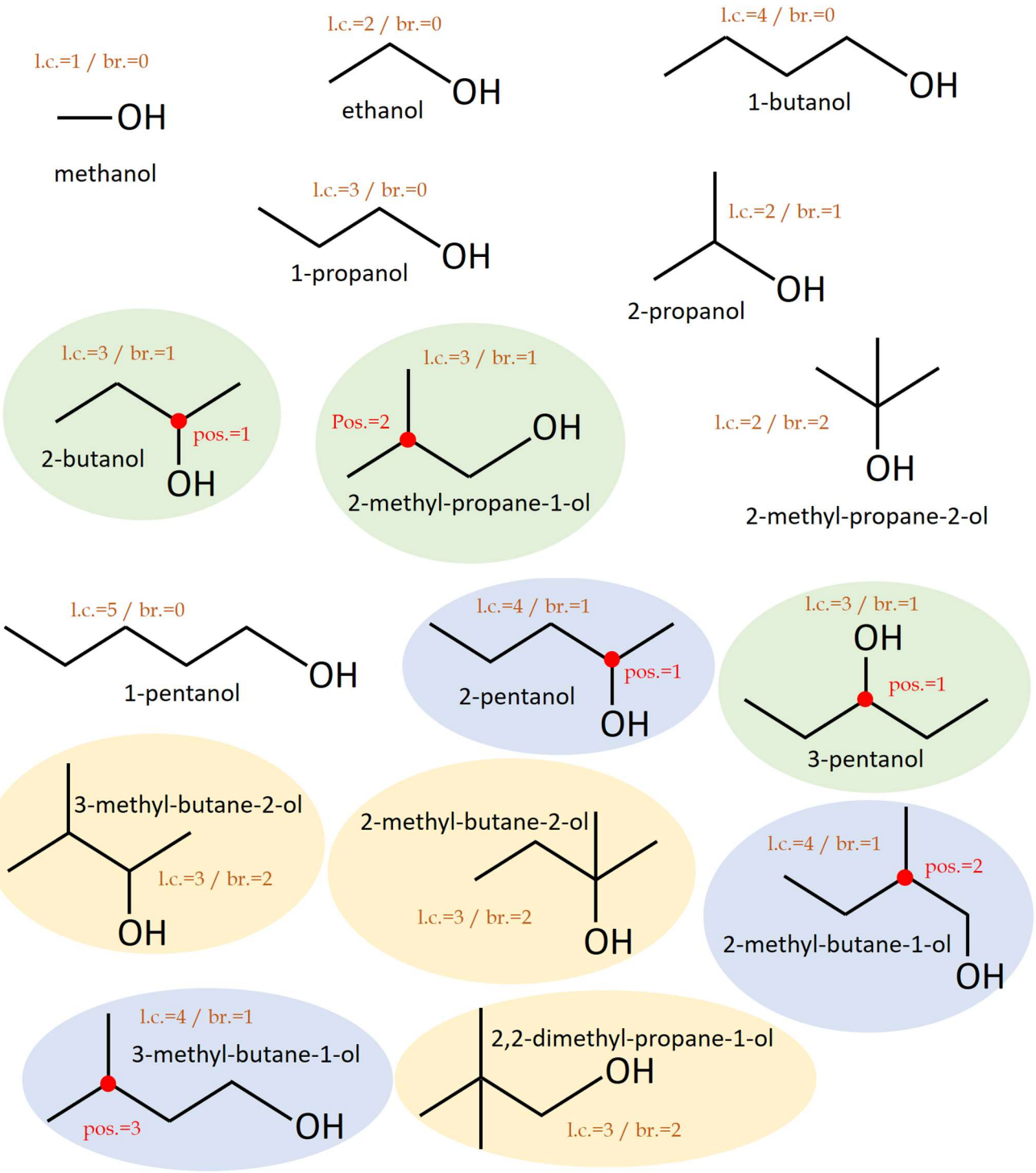


Figure 5: Final digital blackboard showing the development of key figures for the structure of alkanol isomers. Only the structures and names of the alkanols were specified. Abbreviations: l.c. longest chain, br. number of branches, pos. position of branches. Molecules with the same values for l.c. and br. are highlighted in the same color.

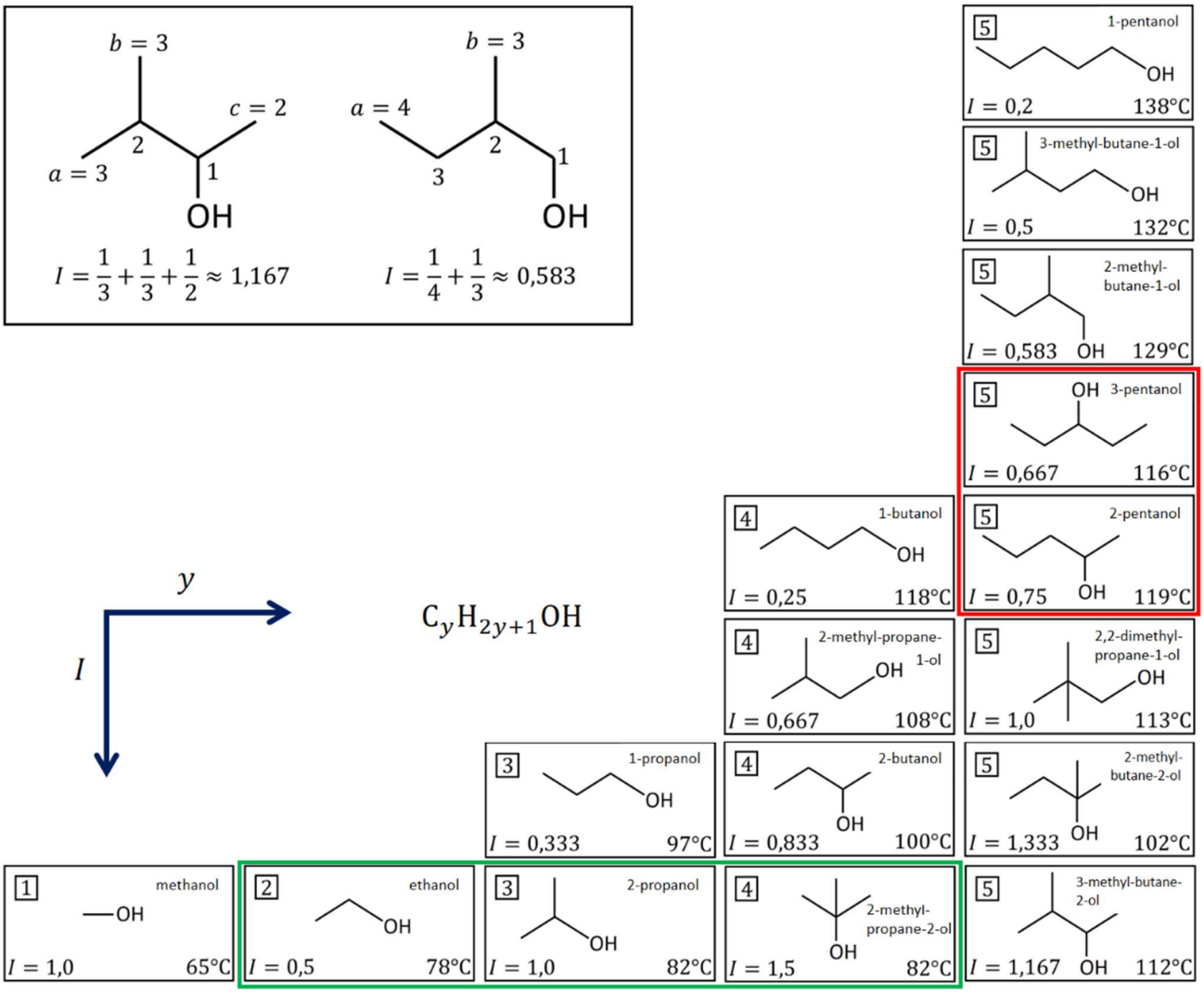


Figure 6: Sorted cards of the alkanols. The green frame shows the student experiments. The red frame marks a deviation in the sequence of boiling temperatures. Inset: Sample calculations for structure index I.

Methanol was omitted here as a borderline case, which improved the correlation of the higher alcohols. Figure 8 also includes data that is not contained in the training data set. This allows check the predictive power of the model. Figure 8a shows that the prediction with this structure index is quite good despite the simple approach. Figure 8b shows the central area enlarged to illustrate the prediction for branched alkanols more clearly.

After regressing the boiling temperatures with index I, the calculation was performed using the index developed by the students (Figure 7b). This showed that the sum of squares error between regression and experiment is slightly higher at 0.0082 than when using I, with a deviation of 0.0029. However, these values are of the same order of magnitude. As stated in the SI, the didactically motivated index developed here and the student index show smaller deviations from the experimental data than individual indices from the sciences. The index developed by the students is therefore of comparable quality in terms of deviations from the experimental data.

As mentioned above, the students used the graphs to identify the relative influence of the carbon number and branching on the boiling point. Their conclusions are confirmed by the resulting correlation equation (see program output in SI) for the plane in Figure 7a:

$$b.p. = \left(-0{,}31438 \cdot \frac{x}{1{,}5} + 0{,}60084 \cdot \frac{y}{5} + 0{,}43110\right) \cdot 138°C$$

Here, x is the structure index I and y is the number of carbon atoms. The data are divided by their maximum values in the data set. This is useful for comparing the weighting of the two influencing factors. The absolute value of $w_2 \approx 0.601$, the weight for the number of carbon atoms, is about twice as large as the absolute value of $w_1 \approx -0.314$, the weight for branching. Thus, the number of carbon atoms has a greater influence. The negative sign of w_1 means that the boiling temperature decreases as branching increases. However, increasing branching lowers the boiling temperature less than an additional CH_2 group raises it

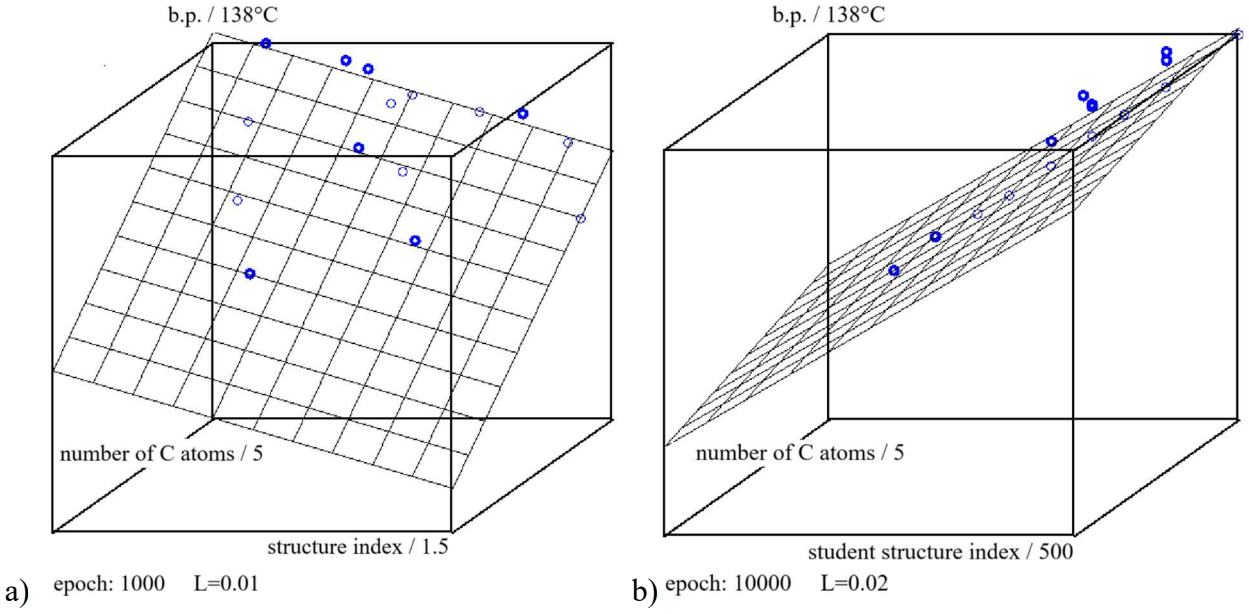


Figure 7: Regression plane for the boiling temperatures of the isomers of alcohols from ethanol to pentanol. The thin circles lie below the plane, the thick circles above it. The values are divided by their maximum values. a) Calculation using the structure index I. b) Calculation using the structure index of the students.

A corresponding analysis of the index developed by the students (Figure 7b) leads to a different conclusion. The parameter $w_1 = 0.641$ is positive, which means that the boiling temperature increases with this structure index. Thus, it does not indicate the degree of branching, but rather the opposite. The value of $w_2 = 0.173$ is significantly smaller than that of w_1. This would mean that branching has a significantly greater influence on the boiling temperature than the number of C atoms. This is because the composition of the indices arbitrarily leads to large jumps due to the ones, tens, and hundreds digits of the three key figures. Even though the student index has a comparatively mean square deviation, its interpretation is less meaningful.

In this final step of the lesson sequence, a complex, differentiated structural model was used to determine the dependence of the boiling point on the degree of branching of the molecules. The structural model represents the molecular interactions and thus enables a satisfactory prediction of the boiling points (Figure 8). This clearly illustrates the relationship between molecular interactions and macroscopic properties. This detailed examination of the subject matter through the application of ML provided the students with numerous opportunities to engage with the chemical content and illustrates that intensive interaction between mathematics and chemistry may be necessary in order to address chemical issues.

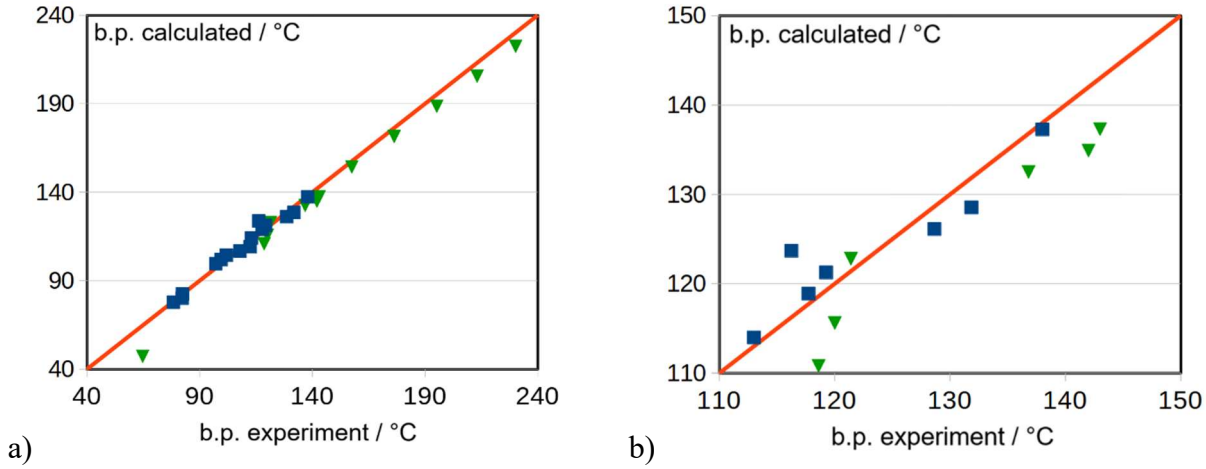


Figure 8: Comparison of correlated boiling temperatures with structure index *I* and experimental values [13]. The diagonal line corresponds to an exact match. The squares are training data, the triangles are predictions. a) The triangles at high temperatures are 1-alkanols, the bottom triangle is methanol. b) Enlarged section of a) (see SI for data).

4. Conclusion

The lesson unit presented here demonstrates how a simplified model of ML, adapted to the requirements of secondary education, can be successfully used to explore a central topic in chemistry teaching, the structure-property relationships of alkanols. The manual approach, including sorting tasks with cards, provided an intuitive introduction to regression analysis, which serves as a bridge to algorithmic modeling.

The activities enabled the students to engage in research-based learning. They actively participated in data analysis by sorting and creating a model for a structure index. In an open and problem-oriented approach, the result of the student structure index was neither predetermined nor steered in a specific direction. The structure index was developed by the students during the discussion and could have turned out differently. The teacher merely moderated in a reserved manner, asked about ambiguities, and recorded the results on the board. The subsequent calculation with the ML program showed the students that their index was well suited. Of course, it is also conceivable that an index developed by students is unsuitable. This then offers the opportunity to discuss the causes. However, the additional index *I* allows the lesson to continue even without a suitable student index.

There were hardly any problems with mathematization in class, which is probably due to the fact that the students had dealt intensively with analysis in parallel mathematics lessons. However, the use of mathematics in chemistry lessons is described as difficult, even if the same content does not cause any problems in mathematics lessons [15-17]. Accordingly, the problem probably lies in the transitions between mathematics and the real situation. It would be helpful here if chemistry teachers had a sound knowledge of mathematics and mathematics education, particularly with regard to mathematical modeling [18] and especially for its application in chemistry lessons [16,17,19].

The lesson unit also has strong links to computational thinking (CT), which can be considered here on two levels. These levels essentially correspond to the definitions of CT [20] according to Papert [21] and Wing [22]. While Papert emphasizes the pedagogical aspect of constructivism, Wing considers CT more from an informatics perspective, defining its ways of thinking as a higher-level thought process that can also be helpful in other subject areas.

The analysis using haptically supported data organization of how molecular structural features influence boiling temperature is consistent with Papert's constructivist approach, in which the active construction and manipulation of "building materials" serves to concretize abstract concepts. The manual method of developing the algorithm, which also starts with

haptic activities and gradually transitions to an algorithm, serves to concretize abstract concepts. The open and problem-oriented learning involved in developing the structure index encourages students to develop and evaluate their own hypotheses, reflecting Papert's emphasis on autonomy and learning through trial and error.

Wing has concretized CT as a strategic approach to problem solving, just as complex questions are converted into simplified algorithms here. This also coincides with Wing's definition, according to which CT describes thought processes for problem formulation and solution through algorithmic representation. The complex topic of structure-property relationships is gradually simplified and abstracted. In general, Wing's CT includes the steps of abstraction, decomposition, algorithm formation, and evaluation and generalization of the results, all of which are included in the teaching unit.

Even though it is emphasized that CT does not necessarily have to lead to programming [20-22], CT is also used pragmatically in chemistry lessons for problem solving. This is creating a code in the sense of Hemmendinger's interpretation [23], according to which people should be allowed to think in their own disciplines and should only be shown how computer science can contribute to solving their problems.

Finally, this article meaningfully combines interdisciplinary content from chemistry, mathematics, and computer science. Although chemistry is clearly in the foreground, the students have learned that contributions from other disciplines can be indispensable. The experience from this and previous learning groups shows that an understanding of interdisciplinarity becomes a matter of course when such approaches are incorporated on a regular basis.

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