COMBINING PAPER-PENCIL TECHNIQUES WITH IMMEDIATE FEEDBACK FOR LEARNING CHEMICAL DRAWINGS

A Thesis

by

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Submitted to the Office of Graduate and Professional Studies of Texas A&M University in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

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August 2019

Major Subject: Computer Science

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ABSTRACT

Introductory chemistry courses teach the process of drawing basic chemical molecules with the use of Lewis dot diagrams. Many beginner students, however, have difficulty in mastering these diagrams. While several computer applications are being developed to help students learn Lewis dot diagrams, there is a potential hidden benefit from paper and pencil that many students may not realize. The goal of this research is to begin identifying which paper-pencil techniques provide educational benefits for learning Lewis dot diagrams. Sketch recognition has been used to identify advanced chemical diagrams, however using the recognition in an educational setting requires focusing beyond identifying the final drawing. This study focuses on creating an effective application that allows students to practice constructing Lewis Dot Diagrams with the same interaction techniques (constructing, checking, and modifying) from pencil and paper, while also providing users informational feedback during the drawing process. Two applications are compared to determine whether including paper-pencil techniques have any educational benefit when drawing Lewis dot diagrams. An analysis of pre-post assessments show how combining sketch recognition of paper-pencil techniques and immediate feedback allows greater benefits for students with a basic chemistry understanding.

ACKNOWLEDGMENTS

I would like to express my gratitude toward everyone who has helped me as I worked on this thesis. Thank you to my advisor, Dr. Tracy Hammond, for giving me the creative freedom to discover this project, and providing me with support and guidance along the way.

Thank you to my committee members, Dr. Theodora Chaspari and Dr. Robert Woodward, for all their advice throughout this project.

Finally, I would like to thank the members of the Sketch Recognition Lab at Texas A&M University, for providing a place of encouragement, and always being available to help.

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1. INTRODUCTION

1.1 Lewis Dot Diagrams

Students who take introductory chemistry classes learn the importance of constructing Lewis dot diagrams. Lewis dot diagrams are structures that show the bonding between atoms of a molecule and the lone pairs of electrons that may exist in the molecule. While these structures seem simple at first glance, they allow us to predict a multitude of molecular properties, and visualize how the molecule is shaped [1]. Figure 1.1 shows an example of how to create the Lewis dot diagram for a chlorine molecule using the electrons available for each atom. Chemical bonding between atoms involve the transfer or sharing of electrons. This transfer or sharing is shown with valence electrons, the outermost electrons of an atom's electron shell. For Lewis dot diagrams, the number of valence electrons for an individual atom is shown with dots that are drawn around the atom. When atoms come together, they form bonds by sharing some of these electrons. These bonds are shown as lines on the diagram [1].



Figure 1.1: The Lewis dot diagram of a chlorine molecule

Introductory chemistry courses teach how to construct Lewis dot diagrams; however, many beginner students have difficulty in mastering them due to the increase in cognitive load that occurs

when they are introduced to the various concepts for different types of diagrams [2]. When the steps for drawing the diagrams become too complex and meaningless, the underlying reason behind drawing the diagrams to understand structural properties of molecules becomes forgotten [3].

1.2 Alternate Learning Methods

Several studies have focused on improving the way students learn Lewis dot diagrams. These studies introduce alternate learning methods that can be used to grasp the concepts of drawing the structures efficiently.

1.2.1 A Focus on Modification

A recently developed method for understanding Lewis dot diagrams teaches students the importance of modifying parts of their diagram [4]. This new focus allows students to remove and move electrons until the final answer is achieved. Similarly, hand held puzzles have also been created to allow students to visualize changing the diagram until the correct molecule is created [5]. These new ideas are emphasizing the practice of editing the diagram, and how removing and moving parts of the molecule are necessary for the learning process in comparison to simply obtaining the correct diagram at first try.

1.2.2 Computer Applications

Educators today are also exploring the use of computer applications in the classroom, and recent research has involved creating applications for students to learn and practice Lewis dot diagrams [6, 7]. These applications allow users to create Lewis dot diagrams on a computer or touch-screen device, while also receiving feedback on the accuracy of their answer. Students can know immediately whether their answer is incorrect, as well as identify what parts of their diagram are incorrect. The immediate feedback that students receive allow them to practice drawing their diagrams more efficiently.

1.3 Chemistry Sketch Recognition

For subjects that involve hand-drawn diagrams, computer applications have implemented sketch recognition to identify and interpret what the user has drawn [8]. Combining sketch recognition with educational applications can have a variety of uses, since many subjects require students to draw diagrams or write out answers to problems. Recent research has also used the concept of sketch recognition to identify and interpret hand-drawn chemical diagrams [9]. Recognizing hand-drawn chemical diagrams is important for advanced chemists, however for educational settings, learning how to draw chemical diagrams requires a different focus. Lewis dot structures are used for teaching and learning how to draw chemical structures. Advanced chemists use shorthand methods to avoid having to draw every single electron in their drawing. Very rarely will you see professional drawings of chemical diagrams use Lewis dot structures. Beginner students, on the other hand, are required to show electrons around each atom, as it reflects their understanding of the molecular structure. Recognizing hand drawn chemical diagrams can be useful for students to check their final answer; however helping students through the new modification methods would require recognizing other techniques.

1.4 Potential Hidden Benefit of Paper Learning

Even though several studies have started to focus on developing computer applications to help students learn Lewis dot diagrams, there is a potential hidden benefit from pencil and paper that many students may not realize. When comparing the effects of online and paper homework, the lack of practicing with handwriting has been shown to contribute to lower scores on exams that test the drawing of complex molecules [10]. While online homework has a clear benefit of providing immediate feedback to users, combining online homework with paper-pencil learning is believed to maximize the learning benefits. As handwriting is found to contribute to motor memory, practicing the action of drawing molecules is important for students to learn Lewis dot diagrams.

1.5 Proposed Work

New methods emphasize the process of constructing, checking, and modifying the structures as more productive for students to learn [11]. This new conceptualization of drawing Lewis Dot Diagrams uses the idea of modification and can be practiced on paper by scratching out and moving parts of the diagram. However, just using this method on paper alone does not provide students with the benefits of immediate feedback. Rather than comparing the final drawing to the correct solution, this study focuses on whether we can create an effective application that allows students to practice constructing Lewis Dot Diagrams with the same interaction techniques (constructing, checking, and modifying) from pencil and paper, while also providing users informational feedback during the drawing process.

The process of constructing, checking and modifying the structures is important for students to learn Lewis Dot Diagrams. This may include erasing or moving parts of the molecule. Beginner students learn the logic behind the process and count electrons as they draw to check their work. When they realize that part of their diagram has an incorrect number of electrons or bonds, they can scratch out and move components, or add missing parts until they reach the correct number. Using sketch recognition, an application for practicing Lewis Dot Diagrams can be implemented such that students are able to use these interaction techniques from paper and pencil. These paper-pencil techniques include drawing lines and dots to add electrons and bonds, circling parts of the diagram to move around electrons or bonds, and scratching out sections to erase electrons or bonds. This study will investigate whether using an application that integrates paper-pencil techniques and immediate feedback results in a stronger ability to draw accurate Lewis Dot Diagrams compared to using an applications, this study addresses the following questions:

1. **Overall Improvement** Will students that use the application with both paper-pencil techniques and immediate feedback experience a greater overall improvement in pre and post quiz scores?

- 2. **Molecule Type Improvement** Will students that use the application with both paper-pencil techniques and immediate feedback perform better on molecules that use multiple bonds?
- 3. **Non-App Molecule Improvement** Will students that use the application with both paperpencil techniques and immediate feedback perform better on molecules that were not practiced on the application?
- 4. **App Interaction Difference** Is there any beneficial difference between the way students interact with the application with both paper-pencil techniques and immediate feedback compared to the way students interact with the application with only immediate feedback.

2. RELATED WORK

This chapter describes the related work for this study in three categories: current methods in teaching Lewis dot diagrams, interactive feedback in developing chemistry computer applications, and benefits of sketch recognition for education and chemistry.

2.1 Recent Methods in Modification

Several studies have involved developing methods for improving students' ability to learn Lewis dot diagrams [12–29]. Some of the new teaching methods have started to focus on the idea of modifying the diagrams. Instead of drawing the correct diagram at first try, these methods encourage the student to obtain an incorrect diagram, and use modification techniques to fix their diagram until the correct structure is achieved. Two of these methods include the Nassiff and Czerwinski Method and Atomic Tiles.

2.1.1 Nassiff and Czerwinski Method

Students experience several difficulties when attempting to learn Lewis dot diagrams [3,30–32]. After recognizing these difficulties in 2015, Peter Nassiff and Wendy A. Czerwinski developed a new method to help students quickly learn the concepts of drawing the correct Lewis structure [4]. While current literature and textbooks focus on filling only outer atoms with electrons [33–36], Nassiff and Czerwinski explain how this type of method causes students to draw incomplete structures when they start counting electrons to check their diagram. Instead, a new method allows students to fill all atoms with electrons rather than just the outer atoms. Generally this causes more electrons to be drawn then required, however, the next steps involve modifying their structure by removing and moving electrons until the correct diagram is achieved. These steps are summarized below.

1. Determine Electrons Determine the total number of electrons needed for the structure.

2. Fill Atoms Give each atom a full octet of electrons (8 for most, ignoring any exceptions)

- 3. **Compare** Compare the number of electrons drawn to the total number of electrons needed from step 1. Determine the number of extra electrons drawn from this comparison.
- 4. **Modify** Remove extra electrons and move electrons to form bonds until all atoms have their full octets again.

Through this method, Nassiff and Czerwinski have emphasized how the practice of editing the diagram to remove and move electrons is necessary for the learning process in comparison to simply obtaining the correct diagram at first try. After examining the use of this method, they concluded that most students were able to master drawing basic Lewis dot diagrams in one classroom session.

2.1.2 Hand-held Portable Tiles

Games and puzzles are commonly used to teach various topics in chemistry [37–39], and handheld model kits have been favored when teaching students to visualize molecular shapes [3]. There is an important focus on helping students increase their representational competence in chemistry [40–44]. While several studies and textbooks highlight the memorization of rules and algorithms [4, 45, 46], these methods are ineffective when students need to gain a strong understanding of pattern recognition techniques that are necessary for advanced chemistry classes [3]. In contrast, a new method similar to puzzles was introduced in 2016. This innovative use of hand-held portable tiles, called Atomic tiles, allows students to increase their knowledge of the necessary pattern recognition techniques.

Atomic tiles are designed so that each tile represents a different atom in a molecule. Around the edges are different combinations of valence electrons, and in contrast to practicing the drawing of Lewis diagrams, the tiles can be moved around until electrons properly connect to other tiles. A final combination of tiles would represent a molecule. Atomic Tiles allow students to try different ideas, move tiles around, and slowly recognize patterns. When analyzing students performance with summative assessments, students who used the Atomic Tiles performed strongly. Since the tiles are designed to encourage students to continuously change the arrangement until they get the correct structure, this study also shows the importance of modification in the learning process of Lewis dot diagrams [5].

2.2 Chemistry Immediate Feedback

Educators today are exploring the use of computer applications in the classroom [47–53]. By using applications that provide feedback, students can immediately know whether their answer is incorrect. This quick gain in knowledge of correctness encourages students to learn how to fix their solution on the spot. Educational applications for chemistry have also started development, as the integration and feedback can benefit students [54–64]. A few of these applications that involve learning Lewis dot diagrams are explained below.

2.2.1 Lewis Dots Touchscreen App

The popularity of touch-screen technologies has caused an increased interest in developing educational applications for both inside and outside of the classroom [65]. Due to their ability to provide a touch enabled interface that encourages interactive learning, tablet applications for education are able to improve engagement and performance [66]. Many touch screen technologies, including iPods and tablets, are positively changing how students learn in the classroom [67–69]. A study in 2012 developed a touch-screen application called "Lewis Dots." Users can select atoms from a toolbar to add them to the screen, and connect available electrons to form molecules. Analysis of the application was designed to include three different modules to assess how effective the iPad application was toward student's learning. Due to the feedback that was immediately present, the application was concluded to be helpful in understanding molecular structures and the use of technology in the classroom did not distract students from learning [6].

2.2.2 OrganicPad Tablet Application

New software is being developed to allow instructors to interact with their students in the classroom. Classroom Presenter [70], Ubiquitous Presenter [71], and Message Grid [72] are all examples of systems where instructors can interact with their students through synchronized presentations and comprehension checks. A system called OrganicPad was created to explore this

idea of instructor-student interaction for chemistry classes [7]. Using TCP/IP communication, students can submit their drawn chemical diagrams. After saving the atoms and their connections as nodes in a graph, these diagrams are then compared to the instructors using graph isomerism to determine whether they are correct. Students can use this immediate feedback to understand how to correct their submission before moving on to next problem. While the immediate feedback that OrganicPad provides is certainly beneficial, this type of design requires an instructors submission to compare solutions with.

2.2.3 Immediate Feedback Problems

In 2015, Smithrud and Pinhas created a study to compare organic chemistry students use of online homework and pencil-paper learning [10]. Grading handwritten homework problems and providing effective feedback is difficult for large class sizes, but online homework can overcome these obstacles by giving immediate feedback and guidance [73]. Online homework has benefited both instructors and students by allowing instructors to monitor student progress, and students have shown a positive attitude and appreciation toward the immediate feedback [74,75].

While online homework has a clear benefit of providing immediate feedback to users, the study believed that our current design of online homework is impeding the way students learn chemistry. When comparing the exam score results in this study, students who used both online homework and paper-pencil learning performed stronger than students who only used online homework. The lack of handwriting may have contributed to some students' poor examination scores. Several other studies have also shown the benefits of learning by handwriting compared to a computer [76–78]. As handwriting is found to contribute to motor memory and learning new symbols [79], practicing the action of drawing and modifying molecules is important for students to learn Lewis dot diagrams.

The application OrganicPad, as explained in section 2.2.2, has taken a step toward using handwriting for developing a more natural interface. Students can draw their solutions as if they were drawing on paper. However, we have not investigated whether including natural modification techniques, such as those explained in section 2.1.1, are also beneficial for students.

2.3 Sketch Recognition

Sketch Recognition involves the automatic identification of handwriting and hand-drawn diagrams. Three general categories separate the different type of algorithms that are used in the field of sketch recognition. These algorithms include gesture-based, geometry-based, and vision-based. Gesture-based algorithms [80–83] focus on interpreting the path of the stroke that is created. In other words, the gesture from pen-down to pen-up is analyzed to determine what is being drawn. Geometry-based algorithms use recognizers [84, 85] to identify general geometrical shapes from a sketch. Vision-based algorithms [86–89] use the sketch as it appears visually instead of focusing on the geometrical aspects of the sketch. This study mainly focuses on the of gesture based features. Using these features, sketches can be trained with machine learning algorithms to be recognized in computer applications.

While sketch recognition can be beneficial for various domains, this study will focus on the related work involved in education and chemistry.

2.3.1 Sketch Recognition in Education

The use of paper and pencil is essential for education, as students are often found to benefit from handwritten notes compared to taking notes on the computer [90]. For subjects that involve hand-drawn diagrams, computer applications have implemented sketch recognition to identify and interpret what the user has drawn. Mechanix, for example, is an educational application that uses sketch recognition to check student's hand-drawn free body diagrams for introductory physics [8, 91–95]. While many online systems have drag and drop features to help learn free body diagrams, Mechanix allows the user to draw the diagrams instead. Using sketch recognition techniques, different components of the drawing can be identified, and the relationship between the drawings can be used to determine the correctness of the diagram. Evaluations of the tool also show that Mechanix is as effective as paper and pencil for learning free body diagrams. Combining sketch recognition with educational applications can have a variety of uses, since many subjects require students to draw diagrams or write out answers to problems.

Sketch Recognition has also been incorporated in electrical engineering by helping students learn to draw digital circuits [96]. Digital Circuit Sketch Recognition (DCSR) is created to allow users to draw circuit diagrams on an application, where immediate feedback is given to output the truth value of the circuit. The DCSR method was shown to perform well for a variety of digital circuits. In addition to digital circuits, sketch recognition of analog circuits have also been beneficial in the education domain [97, 98].

In the field of geography, sketch recognition has been used to build interfaces for students to draw geographical features on a map [99]. By allowing users to draw rivers on a map through an interface, students' work can be quickly evaluated, which would allow them improve their geographic skills more effectively.

2.3.2 Chemistry Sketch Recognition

Recent research has used the concept of sketch recognition to identify and interpret hand-drawn chemical diagrams. In 2011, a new sketch recognition framework called ChemInk was developed for recognizing chemical structures [9]. While the system was able to correctly detect 97.4% of the symbols in a dataset of real-world chemical diagrams, it was geared toward users who already understand how to draw chemical diagrams.

Recognizing hand-drawn chemical diagrams are important for advanced chemists, however for educational settings, learning how to draw chemical diagrams requires a different focus. Lewis dot structures are used for teaching and learning how to draw chemical structures. Advanced chemists use shorthand methods to avoid having to draw every single electron in their drawing. Very rarely will you see professional drawings of chemical diagrams use Lewis dot structures. Beginner students, on the other hand, are required to show electrons around each atom, as it reflects their understanding of the molecular structure. Sketch recognition of complete molecules can be useful for students to check their final answer; however, learning the process of drawing Lewis dot diagrams requires a perspective that involves incorporating modification techniques and immediate feedback. This combination will be discussed in the study methodology in section 3.

3. METHODOLOGY

This chapter discusses the methodology details for the overall study. This includes the outline of each individual experiment, the intervention and observation design, and the evaluation process.

3.1 Study Design

The study will incorporate an OX_1X_2O design, where each participant will have approximately 1 hour to complete the entire study. Figure 3.1 shows how the study is divided. Participants will be selected from undergraduate students at Texas A&M University who only have a introductory knowledge of chemistry concepts. Participants are selected to ensure they have not taken any advanced chemistry courses. Each participant will be randomly assigned to use a version of the application as the treatment. Version one includes the ability to use paper-pencil techniques for editing the molecule, while the second version only has an undo button for editing the molecule. Both versions have the same immediate feedback. Prior to using the application, participants will take a pre-quiz which will include a list of Lewis dot diagrams that need to be drawn. The pre-quiz will also include a general introduction to drawing basic Lewis dot diagrams with a few examples. After the pre-quiz participants will receive a tutorial that will prepare them for using the application for 20 minutes. Once they are finished using the application, the participants will take a post-quiz to determine their improvement in drawing Lewis dot diagrams. In addition to a pre-quiz and postquiz, participants will also take a survey to understand their current chemistry background. The following questions are included on the survey.

- 1. Background What is your Chemistry Background? check all that apply.
 - (a) I have not take any chemistry course prior to this study
 - (b) I have taken a general chemistry class in high school
 - (c) I have taken an advanced chemistry class in high school (Advanced Placement (AP) or

equivalent)

- (d) I have taken a college chemistry course prior to this semester.
- 2. Familiarity How familiar are you with drawing Lewis Dot Diagrams?
 - (a) I have never heard of Lewis Dot Diagrams.
 - (b) I have heard of Lewis Dot Diagrams, but I am not sure what they are.
 - (c) I am familiar with Lewis Dot Diagrams, but I have never used them.
 - (d) I am familiar with Lewis Dot Diagrams, and I have used them.
- 3. **Confidence** On a scale of 1-10, how confident are you in your ability to draw Lewis Dot Diagrams? (1 is not confident, and 10 is very confident)



Figure 3.1: Components of the entire study for each individual participant.

3.2 Treatment Development

As part of the OX_1X_2O design, there are two treatments $(X_1 \text{ and } X_2)$ to create so that their potential effects can be observed. This section describes how these treatments are developed into tablet applications for participants to use.

3.2.1 Deciphering the Basic Lewis Dot Diagram

When using the application, users can complete their drawings of Lewis Dot Diagrams in a sketchpad area. In order to understand the design choices for this area of the application, figure 3.2 shows the breakdown of a basic Lewis Dot Diagram. This breakdown only includes introductory concepts of the Lewis Dot Diagram, and ignores advanced exceptions that are found in more complex molecules. In summary, the components of this breakdown include:

- Central Atom The central most atom in the diagram. This atom is bonded to all other atoms in the diagram.
- Outer Atoms All other atoms around the central atom. Each outer atom is bonded to the central atom.
- Electrons Drawn around an atom. Each atom has four sides, and each side that is not involved in bonding to another atom can contain up to two electrons. Each electron adds one to the electron count for the atom it is drawn around.
- **Bonds** Drawn between atoms, and represents two electrons shared between the atoms. There can be up to three bonds drawn between atoms to connect them. Each bond adds two to the electron count for the atom it is connected to.
- Electron Count The number of electrons an atom uses. The electron count can be calculated by adding each electron around the atom and two times each bond connected to the atom.
- Total Electron Count The total number of electrons drawn in the diagram. The total electron count can be calculated by adding each individual electron drawn and two times each bond

drawn.

- Electrons Needed Each atom's electron count needs to fulfill a certain value to maintain a stable structure for the diagram. The Electrons Needed is generally 8, but some exceptions cause it to be other values. These values become known after practice, however for this study, it is specified with the problem. For the correct diagram to be drawn, the Electron Count for each atom must equal the Electrons Needed specified.
- Electrons Available and Total Available Each atom provides a certain number of electrons to the molecule. The total number of electrons available is the sum of electrons provided by each atom. This number is usually determined by following the periodic table of elements, however for this study, it is specified with the problem. For the correct diagram to be drawn, the Total Electron Count must equal the Total Available.



Figure 3.2: Breakdown of the Basic Lewis Dot Diagram

Each of these components are considered when designing the sketchpad and immediate feedback portions of the application. These designs are explained in sections 3.2.2.1 and 3.2.2.2

3.2.2 Application Design

The tablet application is designed for students to practice drawing the Lewis dot diagram for various molecules. Two versions of the application are created, with one version containing paperpencil techniques, and the other containing an undo button. Both versions have a general molecule page that contains a sketch area with atoms arranged for the molecule, and a feedback area with information about the current drawing. Figure 3.3 shows the layout of the molecule page. In the sketchpad, users can draw bonds between atoms or draw electrons around each atom to complete the Lewis dot diagram. Feedback on the side of the application is provided to help students fix their drawing until it is correct.



Figure 3.3: General Molecule Page Layout

3.2.2.1 Sketchpad

For each molecule in the application, the sketchpad is loaded with the atoms already arranged correctly. In order to complete the diagram, the user just needs to finish drawing the correct bonds and electrons around the atoms. Most introductory chemistry courses also include the concepts of VSEPR theory, which help predict the shape of molecules after drawing the Lewis dot diagrams. Basic Lewis dot diagrams can be described with VSEPR theory [1], and many of the molecules

that don't include advanced concepts or exceptions will have a central atom and 1 to 4 outer atoms. For this reason, the application only used molecules with 2, 3, 4, or 5 atoms. These arrangements are shown in figure 3.4.



Figure 3.4: The application pre-arranges the atoms in each molecule. Each molecule has a central atom, with the remaining atoms surrounding it.

The sketchpad is divided into invisible boxes to guide the user where to draw their bonds and electrons. Anything drawn outside of these boxes is ignored and disappears from the sketchpad. The following guidelines are followed to create these boxes, and Figure 3.5 shows how they are arranged.

- **Bonding Box** The areas between the central atom and outer atoms are bonding boxes. In figure 3.5, these boxes are shown in red.
 - Boxes between the central atom and outer atoms to its right and left are *horizontal bonding boxes*. Boxes between the central atom and outer atoms to its top and bottom are *vertical bonding boxes*
 - Each bonding box can contain up to 3 bonds, so each bonding box is divided into three equal sections. (Horizontal sections for horizontal bonding boxes, and vertical sections for vertical bonding boxes)
 - For each molecule, there are n-1 bonding boxes, where n is the total number of atoms.



Figure 3.5: Bonding and Electron Boxes

- Electron Box The areas on each side of an atom are electron boxes. In figure 3.5, these boxes are shown in green.
 - Any side of an atom that already contains a bonding box will not contain an electron box.
 - Each electron box can contain up to 2 electrons, so each electron box is divided into two equal sections.
 - For each molecule, there are 4n (n 1) electron boxes, where n is the total number

of atoms.

- **Bonding Box Restrictions** Only horizontal lines can be drawn in horizontal bonding boxes. Only vertical lines can be drawn in vertical bonding boxes. The majority of points in a drawn bond must lie in an empty section of a bonding box to be a valid draw and increase the box count.
- Electron Box Restrictions Only small circles or dots can be drawn in electron boxes. The majority of points in a drawn electron must lie in an empty section of an electron box to be a valid draw and increase the box count.
- Box Count Each box keeps count of how many electrons or bonds it is currently holding.

Figure 3.6 shows how bonds and electrons are added to the final boxes. Valid draws are beautified and increase the box count, while invalid draws disappear from the sketchpad. Below the sketchpad is a *clear* button. This clear functionality allows the user to remove all bonds and electrons from the boxes and reset all box counts to 0.

3.2.2.2 Feedback

On the right side of the molecule page is a feedback area. When the user clicks on the *check* button below the sketchpad, the application analyzes the sketchpad to evaluate whether the drawn diagram is correct. The feedback area shows which parts of the diagram are correct based on three major checks: Connected, Full Octets, and Total Electrons. These checks are explained below.

- **Connected** All atoms must be connected. In order to check this, every bonding box in the sketchpad must contain at least one bond. Since each box keeps track of the number of bonds or electrons it contains, the Algorithm 1 is used to check if Connected is true:
- Full Octets Each individual atom must have the correct number of electrons needed, which is specified in the problem given. As explained in section 3.2.1, this refers to how the Electron Count for each atom must equal the Electrons Needed specified. The Electron Count is



Figure 3.6: Valid bond and electron sketches are beautified and added to their final boxes.

calculated by counting each bond and electron around the atom. 2 electrons are added for each bond, and 1 electron is added for each electron. Algorithm 2 shows how each atom is checked for this equality.

• **Total Electrons** The total number of electrons in the diagram must match the total electrons needed, which is specified in the problem given. As explained in section 3.2.1, this refers to how the Total Electron Count must equal the Total Electrons Available specified. The Total Electron Count is calculated by counting each bond and electron drawn for the entire diagram. 2 electrons are added for each bond, and 1 electron is added for each electron.

Algorithm 1 Connected

for each box do
 if box.type == "bonding" then
 if box.count == 0 then
 return false
 end if
 end if
 end for
 return true

Algorithm 2 Full Octet

```
for each atom do
  electronCount = 0
for each box attached to atom do
    if box.type == "bonding" then
      electronCount+ = 2 * box.count
    else
      electronCount+ = box.count
    end if
end for
if electronCount == atom.electronNeeded then
    report correct for atom
end if
end if
end for
if end for
```

Algorithm 3 explains how to check the total electrons.

Algorithm 3 Total Electrons

totalElectronAvailable = 0for each atom do total Electron Available + = atom. electron Availableend for totalElectronCount = 0for each box do if box.type == "bonding" then totalElectronCount + = 2 * box.countelse totalElectronCount + = box.countend if end for **if** totalElectronCount == totalElectronAvailable **then** return true else return false end if

3.2.2.3 Sketch Recognition

In order to recognize sketches for the application, sketch recognition would need to be implemented for recognizing lines for bonds, dots for electrons, larger circles for moves, and scribbles for removes. Previous methods of gesture recognition have been studied by Dean Rubine, who created a recognition method in 1991 [81]. By selecting a number of features and analyzing them with a linear classifier, this method has the ability to recognize a gesture with high accuracy. Only four simple gestures need to be identified for this study, and since pairing Rubine's features with a classifier has shown to recognize gestures with high accuracy, all 13 features are implemented. Appendix A lists each of these features with a label that explains how they are related to a sketch.

The application is setup so that training sketches are collected for each participant through a tutorial page. The different tutorials are explained in section 3.2.3. When the user draws a sketch

on the main application pages, a decision tree is used to classify the sketch as a bond, electron, move, or remove. The steps to handle a valid recognition are also explained in 3.2.3.

3.2.3 Treatment Types

Since there are two treatment types for this experiment, two application versions are created. The general sketchpad design and feedback are consistent between the two application versions. The main difference lies in the ability to modify the diagram drawn in the sketchpad. Version 1 uses paper-pencil techniques that allows the user to edit specific parts of the diagram, while Version 2 has an undo button to remove the previous sketch.

3.2.3.1 Application Version 1

In order to assess whether integrating pencil-paper techniques improves the ability to draw Lewis dot diagrams, the different techniques are first determined. The process of constructing, checking and modifying the structures are important for students to learn Lewis Dot Diagrams [11], so these three categories are chosen as a basis for the techniques. Similarly, the method by Nassiff and Czerwinski show the importance of removing and moving electrons and bonds until the correct diagram is achieved [4]. The three techniques are finalized as drawing, moving, and removing:

- 1. Drawing—Drawing bonds and electrons with lines and dots
- 2. Moving—Circling bonds or electrons and redrawing them at a different location
- 3. Removing—Scribbling over bonds and electrons to erase them

To integrate paper-pencil techniques to the sketchpad, the tutorial section is modified to allow users to add the techniques of moving and removing. The tutorial section adds four pages to collect training data: Remove Bonds, Remove Electrons, Move Bonds, and Move Electrons.

- Training: Remove Bonds and Remove Electrons
 - The user scribbles over individual bonds and electrons to make them disappear. The scribble sketches are first checked to ensure a majority of the points lie in an individual

box that is not empty. Valid scribbles are saved in the training data with an interpretation label "remove."

- Training: Move Bonds and Move Electrons
 - The user circles individual bonds and electrons, and redraws them in a different location. The circle sketches are first checked to ensure the points are surrounding an individual box that is not empty. Valid circles are saved in the training data with an interpretation label "move."

In addition to modifying the tutorial section, the sketchpad on the main application page is updated to include the ability to edit the diagram with these new techniques. When a sketch is recognized as a "remove" or a "move", then the sketchpad follows these steps:

- Remove Recognized
 - The "remove" sketch is checked to ensure that a majority of points from the sketch lies in an individual box that is not empty. This causes only one bond or electron to be removed at a time.
 - Valid "remove" sketches modify the sketchpad so that the electron or bond under the "remove" sketch disappears.
 - The box count for the designated box that the remove occurred in decreases by 1.
- Move Recognized (Individual Electron/Bond)
 - The "move" sketch is checked to ensure that a majority of points from the sketch surrounds an individual box that is not empty. This causes only one bond or electron to be moved at a time.
 - Valid "move" sketches modifies the sketchpad so that the electron or bond within the "move" sketch turns grey.

- An "X" cancel button appears on the top right to allow the user to cancel the move action. Otherwise, the sketchpad waits for the user to redraw the selected electron or bond to another location.
- If an electron is selected, then the user can only redraw in electron boxes. If a bond is selected, then the user can only redraw in bonding boxes. Once redrawn, the grey electron or bond disappears from the sketchpad.
- Move Recognized (Two Electrons)
 - As shown in the modification method developed by Nassiff and Czerwinski, it is common to move two electrons into a bond [4]. For this reason, the ability to move two electrons is created.
 - The "move" sketch is checked to ensure that a majority of points from the sketch surrounds a main electron box that contains two electrons.
 - Valid "move" sketches modifies the sketchpad so that the electron pair within the "move" sketch turns grey.
 - An "X" cancel button appears on the top right to allow the user to cancel the move action. Otherwise, the sketchpad waits for the user to redraw the selected electron or bond to another location.
 - If the user redraws in another electron box that is empty, then both electrons are moved to that location. If the user redraws in an individual bonding box that is empty, then a bond is created while the original electron pair disappears from the sketchpad.

3.2.3.2 Application Version 2

The second version of this application appears very similar to the first version, with the exception of an undo button. Electron and bond sketches are collected in the tutorial for the training data, however technique sketches for modification are not included in this version. Instead, the user has an undo button to remove any previously drawn sketches. The molecule questions and the immediate feedback for this version remains the same as the first version.

The main functionality of the undo button is to remove the previously drawn sketch. To set up this ability, the sketchpad keeps track of each bond and electron drawn. Since each bond and electron has an individual box where it can be stored, these boxes are first numbered. When a box is filled with a drawn bond or electron, its number is added to a list for the undo button to use. When a user clicks on the undo button, the list is used to remove a sketch. First, the last box number in the list is obtained as it refers to the most recent bond or electron drawn. This box's bond or electron is removed from the sketchpad, and the main box count for this box decreases by one. Finally, the box number is removed from the list.

3.3 Observations

For the OX_1X_2O design of the study, the observations include a pre-quiz that is taken before the application, and post-quiz that is taken after the application. During application usage, data is collected to understand how the participants interact with the application. This section explains how the quizzes are designed for consistency, how they are graded for analysis, and how the application data will be collected and used for evaluation.

3.3.1 Quiz Design

To observe the effects of the two treatments, participants will complete a pre-quiz prior to using the application, and a post-quiz after using the application. The assessment will consist of drawing the Lewis dot diagrams for 20 different molecules that range in difficulty. Students will have 12 minutes to complete as many Lewis dot diagrams as they can. A general introduction with basic examples will be provided with the quizzes to allow students to reference as they complete the quiz.

3.3.1.1 Determining Diagram Complexity

Before creating the quizzes, the complexity of molecules were analyzed to help create a balance of difficulty. As there are three types of bonding, there are three different types of molecules that
can be drawn. Lewis dot diagrams can show molecules with single bonds, double bonds, and triple bonds. Figure 3.7 shows how the modification method by Nassiff and Czerwinski requires increasing modification techniques as the number of bonds increase. A molecule with just single bonds can usually be obtained without any modifications. A molecule with double or triple bonds, however, will require additional removals and moves to form the multiple bonding. This causes the complexity of the molecule to increase when trying to draw the complete Lewis dot diagram. Section 3.3.1.2 and 3.3.2 explains how this complexity is taken into consideration for designing the quiz, as it effects the analysis.

Н — Ö́ — Н	: Ö − Ö: : Ö − Ö: : Ö − O: : Ö = O:	$:\ddot{C} - \ddot{O}:$ $:\ddot{C} - \ddot{O}:$ $:\ddot{C} - O:$ $:\ddot{C} - O:$ $:C = O:$ $:C = O:$ $:C = O:$
Electrons Available:	Electrons Available:	Electrons Available:
O: 6, H: 1, H: 1, Total: 8	O: 6, O:6, Total: 12	C: 4, O:6, Total: 10
Electrons Needed:	Electrons Needed:	Electrons Needed:
O: 8, H:2 , H:2	O: 8, O:8	C: 8, O:8
Step 1: Give each atom Electrons Needed. (Total Electron Count = 8, Total Electrons Available = 8) O Modifications Used	Step 1: Give each atom Electrons Needed. (Total Electron Count = 14, Total Electrons Available = 12) Step 2: Remove 2 electrons. (Total Electron Count = 12, Total Electrons Available = 12) Step 3: Move 2 electrons. (Electrons Needed Correct) 2 Modifications Used	Step 1: Give each atom Electrons Needed. (Total Electron Count = 14, Total Electrons Available = 10) Step 2-3: Remove 4 electrons. (Total Electron Count = 10, Total Electrons Available = 10) Step 4-5: Move 4 electrons. (Electrons Needed Correct) 4 Modifications Used

Figure 3.7: Diagram Complexity: Modifications needed increase as the number of bonds increase.

3.3.1.2 Quiz Layout

Both the pre-quiz and the post-quiz contain 20 different molecules. These molocules were chosen from the commonly tested Lewis structures [100]. Due to the range of complexity found in molecules, as discussed in section 3.3.1.1, a similar number of molecules are used for each bonding type. Molecules with single bonds are labeled as easy, double bonds are labeled as medium, and triple bonds are labeled as hard. Any double bonded molecule that had the additional challenge of considering its charge was moved up to the hard label. With this organization, 7 molecules are easy, 6 are medium, and 7 are hard. Since several molecules between the two quizzes are the same, the layout of the quiz is created so that molecules can be reorganized. For both quizzes, the placement of molecules based on their difficulty levels remains consistent. Thus, where an easy molecule is located on the pre-quiz, a different easy molecule. In addition to maintaining the layout between quizzes, each row of the quiz also contains a mix of easy, medium, and hard molecules. This decision was made to try influencing participants to attempt a range of difficult molecules. However, the participant still has the ability to skip to different molecules around the quiz, if they choose to do so.

3.3.1.3 Non-App Molecules

Between taking the pre-quiz and post-quiz, participants use an application that allows them to practice 22 different molecules. These molecules can be connected to the molecules on the quizzes, either by having the exact same atoms, or by having a similar structure. When taking the post-quiz, participants will be drawing their answer to many similar molecules that they have had practice drawing on the application. However, a few post-quiz molecules are not connected to any of the application molecules. These molecules are labeled as "Non-App Molecules," as participants will not have practice seeing how their structures are completed. Table 3.1 shows the connection between quiz and app molecules, as well as which post-quiz molecules are labeled as Non-App molecules.



Figure 3.8: While molecules are rearranged, the quiz layouts remain consistent between pre and post by keeping the placement of easy, medium, and hard molecules.

3.3.2 Quiz Grading

To analyze the improvement between quizzes, a consistent grading system was created to score each molecule on the quiz. To go beyond simply right and wrong, the Lewis dot diagrams were analyzed to determine how far off a student was from the correct answer. The following guidelines were used for a consistent grading process:

• Molecule Value Each molecule has a total value that is dependent on the type of molecule, or whether it is a non-app molecule. These values are used when grading the pre and post quizzes. As explained in section 3.3.1.1, the complexity of molecules increases as the number of bonds increase. This is taken into consideration by giving molecules with

Pre-Quiz			Post-Quiz		
easy	medium	hard	easy	medium	hard
HCl	O2	HNO3	HF	O2	HNO3
H2O	CH2O	NO3-	H2O	CH2O	NO3-
OF2	CS2	NO2-	OF2	CS2	NO2-
CH4	CO2	СО	CH4	CO2	СО
PH3	SO3	N2	NH3	SO3	N2
SCl2	C2H4	HCN	SC12	C2H4	HCN
BF3		C2H2	NH2OH		C2H2

Table 3.1: List of Quiz Molecules with their Difficulty Level. Bold molecules on the post-quiz are Non-App molecules.

triple bonds a higher molecule value than molecules with double bonds, which will have a higher molecule value than molecules with single bonds. Non-app molecules on the post quiz have the highest value. Since these molecules have never been practiced on the app, as explained in 3.3.1.3, their solutions will be new to participants. These molecules show a stronger understanding of concepts, and have been given the highest molecule value on the post-quiz.

- **Correct** If a Lewis dot diagram is drawn correctly, then the student is awarded the Molecule Value for that molecule.
- Incorrect Bonds/Electrons
 - Incorrect: Extra/Missing Bond For each extra or missing bond, 1 point is subtracted from the Molecule Value.

- Incorrect: Extra/Missing Electron For each extra or missing electron, 1/2 point is subtracted from the Molecule Value.
- Incorrect, but Correct Total Electrons As explained in section 3.2.1 when deciphering the Lewis dot diagram, a correct diagram requires the Total Electron Count to equal the Total Available. So if a diagram is overall incorrect, but the total electrons used in the diagram is still correct, then 1 point is awarded back.
- Incorrect, but Correct Individual Atom As explained in section 3.2.1 when deciphering the Lewis dot diagram, a correct diagram requires each atom's Electron Count to equal the Electrons Needed. For each atom that has the correct number of electrons used, 1/n point is awarded back, where n is the total number of atoms.
- Incorrect Max Score/Min Score When points are taken off or given back, a minimum and maximum score are followed to ensure scores are not negative or over the full score. When a molecule is incorrect, the final score calculate is compared against 0, and any score below is replaced with 0. The final score is also compared against (Molecule Value 0.5), and any score above this is replaced with (Molecule Value 0.5).
- **Incorrect Arrangement** If a molecule has atoms incorrectly arranged, or bonds and electrons are placed in areas where they are not allowed
 - Incorrect, but Correct Total Electrons and Correct Individual Atoms Only half of the Molecule Value is awarded.
 - Incorrect No points
- Not Attempted Blank answers where participants did not attempt the molecule are awarded 0 points.

Using the grading system above, the total points awarded for the whole quiz is calculated, as well as the total points for each molecule type and new molecules. Figure 3.9 shows an example of how the grading system results in different scores for various incorrect answers.



Figure 3.9: Examples of Different Score Results from Grading

3.3.3 Application Data

As each participant in the study uses the application, a table is created to observe how they interact with their version of the app. For each molecule, the following information gets collected:

- The number of "removes" drawn. (version 1 only)
- The number of "moves" drawn. (version 1 only)
- The number of times the undo button is clicked. (version 2 only)
- The number of times the clear button is clicked.

- The number of times the check button is clicked.
- The time it takes to finish the molecule.

Through this process, the total time and the number of molecules completed is also collected.

3.4 Evaluation

Four questions are addressed in this study, and are analyzed based on the quiz scores and the way students interacted with each application version. These questions are listed below.

- 1. **Overall Improvement** Will students that use the application with both paper-pencil techniques and immediate feedback experience a greater overall improvement in pre and post quiz scores?
- 2. **Molecule Type Improvement** Will students that use the application with both paper-pencil techniques and immediate feedback perform better on molecules that use multiple bonds?
- 3. **Non-App Molecule Improvement** Will students that use the application with both paperpencil techniques and immediate feedback perform better on new molecules that were not practiced on the application?
- 4. **App Interaction Difference** Is there any beneficial difference between the way students interact with the application with both paper-pencil techniques and immediate feedback compared to the way students interact with the application with only immediate feedback.

3.4.1 Overall Improvement

For each version of the app, the post-quiz scores and pre-quiz scores are compared using a Mann Whitney U Test to determine if there is a significant improvement. In order to determine if there is a difference in overall improvement between the two versions of the app, the difference between the pre-quiz and post-quiz score is calculated for each participant. The quiz score differences are then compared using a Mann Whitney U Test with an alpha value of 0.05 to see if one version has a stronger improvement compared to the other.

3.4.2 Molecule Type Improvement

To analyze how the app versions differed in molecule type improvement, the scores are divided up into three different categories for each molecule type. The total score in each category is used as a pre and post score. The difference between these scores are compared using a Two Sample T Test and a Mann Whitney U Test to see if one version has a stronger improvement compared to the other. Additionally, the average post score values for each molecule can show use which molecules caused participants to struggle. From these values, we can determine which app version resulted in lower scored molecules.

3.4.3 Non-App Molecules

For the six non-app molecules on the post-quiz, the post score values for each molecule is used to show which molecules had lower scores. Using a Mann Whitney U Test, we can determine if an one app version had significantly more lower scored non-app molecules than the other.

3.4.4 App Interaction Difference

Using the data collected from the application, Mann Whitney U Tests and Two Sample T Tests are used to see if there are any significant differences between the way students interacted with the application. The total time, average time per molecule, total techniques/undos, total clears, total checks, and total molecules completed are compared between each application.

3.4.5 Sketch Recognition Analysis

In addition to evaluating the four questions from the study, the accuracy of the sketch recognition implemented in the application is also analyzed. Since training sketches are collected for each participant through the tutorial page, the accuracy of the recognition method can be analyzed using Leave One Out Cross Validation. Each participants sketches that are inputted into the tutorial page are tested using a decision tree classifier, where the remaining participants' tutorial sketches are used as training data. Using the 13 Rubine features listed in appendix A, the output of the decision tree can be used to create a confusion matrix of which gestures are identified correctly.

4. RESULTS

This chapter presents the results from analyzing quiz scores and app interaction. These results are presented in five categories: overall improvement, app molecule type improvement, non-app molecule scores, app interaction difference, and sketch recognition accuracy. A total of 15 participants were recruited for the study, where 7 used the application with paper-pencil techniques and the other 8 used the application with the undo feature.

4.1 Survey Results

Before taking the pre-quiz, participants completed a survey to understand their current chemistry background, familiarity, and confidence. The results for the three questions are presented in this section.

4.1.1 Background

To assess the current background of participants, the first survey question asked what types of chemistry courses have been taken in the past.

- 1. What is your Chemistry Background? check all that apply.
 - (a) I have not take any chemistry course prior to this study
 - (b) I have taken a general chemistry class in high school
 - (c) I have taken an advanced chemistry class in high school (Advanced Placement (AP) or equivalent)
 - (d) I have taken a college chemistry course prior to this semester.

All 15 participants have at least taken a high school chemistry course. Using the answers given, two categories of chemistry background were created: high school only and college. Participants who circled b or c alone, or both b and c, were categorized as only having a high school background in chemistry. Participants who included choice d were categorized as having a college background.

As figure 4.1 shows for this study, 8 participants have only a high school background, while 7 participants have a introductory college background.



Figure 4.1: Chemistry Background Survey Results

4.1.2 Familiarity

The next survey question asked how familiar participants were with Lewis dot diagrams.

- 1. How familiar are you with drawing Lewis Dot Diagrams?
 - (a) I have never heard of Lewis Dot Diagrams.
 - (b) I have heard of Lewis Dot Diagrams, but I am not sure what they are.
 - (c) I am familiar with Lewis Dot Diagrams, but I have never used them.
 - (d) I am familiar with Lewis Dot Diagrams, and I have used them.

While each response suggests that everyone has heard of Lewis dot diagrams, not every participant has the experience of using them. Figure 4.2 presents the results from this question in three categories. Those who answered choice b were categorized with some familiarity, and participants who answered choice c or d were categorized with familiar but never used, or familiar and used respectively.



Figure 4.2: Chemistry Familiarity Survey Results

4.1.3 Confidence

The final survey question asked how confident participants felt with drawing Lewis Dot Diagrams.

 Confidence On a scale of 1-10, how confident are you in your ability to draw Lewis Dot Diagrams? (1 is not confident, and 10 is very confident)

Participants who answered with a level between 1-3 were categorized with having low confidence, 4-6 were categorized with having some confidence, and 7-10 were categorized with having high confidence. Figure 4.3 shows how all 15 participants responded to confidence level, as well as how confidence levels were divided with each application version.

4.2 **Overall Improvement Results**

Both the pre-quiz and post-quiz have 20 molecules, where the single-bonded molecules are worth 5 points, double-bonded molecules are worth 8 points, and triple-bonded molecules are worth 10 points. The post-quiz also contains non-app molecules that are worth 15 points. This scoring system caused the pre-quiz to have a total of 153 points and the post-quiz to have a total of 192 points. The final score for each participant was calculated as a percentage.



Figure 4.3: Chemistry Confidence Survey Results

4.2.1 Individual Quiz Scores

Table 4.4 shows the pre-quiz score, post-quiz score, and score differences for each of the 15 participants. Figure 4.5 shows the overall quiz score change for each application version, which explains how the average pre-quiz to post-quiz score change differs between both applications.

	Paper-Pencil Techniques				Undo		
	pre-quiz	<u>post-quiz</u>	score difference		pre-quiz	post-quiz	score difference
	31.5	62.41	30.91		63.29	74.53	11.24
	79.08	89.84	10.76		87.91	79.17	-8.74
	39.61	52.60	13.00		65.69	74.57	8.88
	38.24	75.39	37.16		77.48	84.95	7.46
	56.21	100	43.79		40.03	67.76	27.73
	85.29	92.86	7.57		47.93	64.06	16.13
	40.31	78.13	37.82		27.65	37.76	10.11
					53.04	61.59	8.55
average	52.89	78.75	25.86	average	57.87	68.05	10.17
standard error	7.5	5.95	5.24	standard error	6.53	4.79	3.34

Figure 4.4: Quiz Score Results for 15 Participants



Figure 4.5: Overall Quiz Score Change

4.2.2 Statistical Analysis of Quiz Scores

To analyze whether one application has a significantly stronger improvement than the other, the quiz scores and score differences are compared using a one-tailed two sample t-test with a significance level of 0.05. However, because of the small sample size, a non-parametric test (Mann-Whitney U Test) is also used to compare the quiz scores and score differences. The non-parametric tests are also set up as a one-tailed test with a significance level of 0.05. Table 4.1 shows the resultant p-values and u-values for comparing both applications' pre-quiz scores, post-quiz scores, and score differences.

4.2.3 Quiz Scores by Chemistry Background

Using the survey results from section 4.1, the overall results were also divided between chemistry background. To visualize any difference between those who had a college background of introductory chemistry and those who had a high school background of introductory chemistry, figure 4.6 and table 4.2 show the quiz score differences between the two categories.

Pre-Quiz Comparison		Post-Quiz Comparison		Score Difference Comparison	
One-Tailed Mann Whitney U Test		One-Tailed Mann Whitney U Test		One-Tailed Mann Whitney U Test	
U Value (Undo)	23	U Value (Undo)	39	U Value (Undo)	45
U Value (Paper-Pencil)	33	U Value (Paper-Pencil)	17	U Value (Paper-Pencil)	11
Critical U (0.05 significance level)	13	Critical U (0.05 significance level)	13	Critical U (0.05 significance level)	13
One-Tailed Two Sample T Test		One-Tailed Two Sample T Test		One-Tailed Two Sample T Test	
p-value	0.3234	p-value	0.1053	p-value	0.0158

Table 4.1: Two Sample T-Test and Mann-Whitney U Test Results for Comparing Pre-Quiz Scores, Post-Quiz Scores, and Score Differences



Figure 4.6: Quiz Score Change for High School Background and College Background of Introductory Chemistry

4.3 App and Non-App Molecule Type Improvement

Each of the molecules on the pre-quiz and post-quiz were graded based on their difficulty level. Molecules that were practiced on the application were valued based on the number of bonds they used. Single-bonded molecules are worth 5 points, double-bonded molecules are worth 8 points, and triple-bonded molecules are worth 10 points. The molecules that were not practiced on the application are worth 15 points on the post-quiz. Each molecule's score is calculated as a percentage.

High School Only					College			
				(0				
	Pre-Quiz	Post Quiz	Score Difference	due		Pre-Quiz	Post Quiz	Score Differen
	31.5	62.41	30.91	chni		79.08	89.84	10.76
	39.61	52.6	13	ITe		56.21	100	43.79
	38.24	75.39	37.16	enci		85.29	92.86	7.57
	40.31	78.13	37.82	er-P				
				Pap	Average	73.53	94.24	20.71
Average	37.41	67.13	29.72					
	Pre-Quiz	Post-Quiz	Score Difference			Pre-Quiz	Post-Quiz	Score Differen
	40.03	67.76	27.73			63.29	74.53	11.24
	47.93	64.06	16.13	유		87.91	79.17	-8.74
	27.65	37.76	10.11	Uno		65.69	74.57	8.88
	42.16	57.79	8.55			77.48	84.95	7.46
Average	38.54	56.53	17.99		Average	73.59	78.3	4.71

Table 4.2: Pre-Quiz and Post Quiz Scores for High School and College Background of Introductory Chemistry

4.3.1 Post-Quiz Scores by App Molecule Type

After using the application, each participant took a post-quiz with the same molecules. The score for individual molecules are calculated for each participant, and averaged for each type of application. Using the molecules that were practiced on the application, figure 4.7 shows the average post-quiz score for each molecule on both versions of the application. The molecules that scored 80% or below are highlighted in red.

4.3.2 Quiz Score Change by App Molecule Type

The application versions are also compared by the quiz score difference for each molecule type practiced on the application. In addition to an overall score, each participant has a score for each molecule type (easy, medium, and hard). The average pre-quiz and post-quiz scores by molecule type are shown in figure 4.8, where the change from pre-quiz to post-quiz are displayed for each application version.



Figure 4.7: Molecule Type Post Quiz Scores for Paper-Pencil Technique Application and Undo Application



Figure 4.8: Molecule Type Score Change

4.3.3 Non-App Molecule Type Scores

The molecules that were not practiced on the application are worth 15 points on the post-quiz. The score for individual non-app molecules are calculated for each participant, and averaged for each type of application. Figure 4.9 shows the average post-quiz scores for the non-app molecules on both versions of the application. The molecules that scored below 80% are highlighted in red.



Figure 4.9: Non-App Molecule Post Quiz Scores for Paper-Pencil Technique Application and Undo Application

4.3.4 All Type Molecule Scores

Post-quiz scores for all participants include easy (single-bonded), medium (double-bonded), hard (triple-bonded), and non-app molecules. To summarize the differences between application types, the individual molecule averages in each category from section 4.3.1 and section 4.3.3 are averaged together. The post-quiz averages for each molecule type are shown in figure 4.10.

4.4 Weighted All-or-Nothing Quiz Scores

Since the overall improvement from section 4.2 is dependent on the values given to each molecule, it is beneficial to show the results from weighting the molecules in an all-or-nothing method. In this grading approach, only molecules that are drawn completely correct are awarded its molecule value, while the remaining molecules are given no points. Results from this grading



Figure 4.10: All Molecule Type Post Quiz Scores for Paper-Pencil Technique Application and Undo Application

method show which application scored higher for fully correct molecules. Figure 4.11 shows the overall quiz score change for each application version, which explains how the average pre-quiz to post-quiz score change differs between both applications, when using an all-or-nothing grading method. This grading method is also used to show the post-quiz scores by molecule type in figure 4.12, and the non-app post-quiz scores in figure 4.13. For these figures, molecules that scored 70% or below are highlighted in red. This cutoff was decreased as the overall scores were generally lower in this category due to the removal of partial credit.

4.5 App Interaction Difference

While participants use each version of the application, data is collected to analyze how users interact with the application. This data includes the total number of techniques used (remove and move / undo), total number of times the clear button is used, total number of time the check button is used, total number of molecules completed, and the average time spent per molecule. Figure 4.14 shows the average of these values from each version of the application.



Figure 4.11: Quiz Score Change with All-or-Nothing Grading Method

A one tailed Mann-Whitney U Test with a significance level of 0.05 is used to compare the app interaction between paper-pencil techniques and the undo application. The resultant U values are shown in table 4.3.

	total techs/undo	total clears	total checks	total molecules done	avg time/molecule
U-value (Paper-Pencil Techniques)	31.5	30	24	32	21
U-value (Undo)	17.5	19	25	17	28

Table 4.3: Mann-Whitney U Test Results for Comparing Paper-Pencil Techniques and Undo App Interaction



Figure 4.12: Molecule Type Post-Quiz Scores with All-or-Nothing Grading Method

4.6 Sketch Recognition Accuracy

A Leave One Out Cross Validation is used to test each participant's tutorial sketches with a decision tree classifier, where the remaining participants' sketches are used as training. Each participant that used the paper-pencil techniques application is required to draw 12 bonds, 24 electrons, 36 removes, and 18 moves. Each participant that used the undo application is required to draw 12 bonds and 24 electrons. For 15 participants, where 7 used paper-pencil techniques and 8 used the undo application, a total of 180 bonds, 360 electrons, 252 removes, and 126 moves are drawn.

The total confusion matrix created from the Leave One Out Cross Validation is shown in table 4.4, and the individual decision trees generated are listed in appendix A. The results from the confusion matrix are also analyzed by calculating the sensitivity, specificity, false negative rate, and false positive rate for each individual gesture. These values are shown in 4.5.



Figure 4.13: Non-App Molecule Post-Quiz Scores with All-or-Nothing Grading Method



Figure 4.14: App Interaction of Paper-Pencil Techniques vs Undo Application

	Bond	Electron	Remove	Move		Bond	Electron	Remove	Move
Bond	175	1	4	0	Bond	0.972	0.0056	0.022	0
Electron	2	337	19	2	Electron	0.0056	0.936	0.0528	0.0056
Remove	4	15	221	12	Remove	0.0159	0.0595	0.877	0.0476
Move	1	0	7	118	Move	0.00794	0	0.0556	0.937

Table 4.4: Leave One Out Cross Validation Confusion Matrix of Bond, Electron, Remove, and Move Sketches

	Sensitivity	Specificity	False Negative Rate	False Positive Rate
Bond	0.972	0.991	0.028	0.0095
Electron	0.936	0.971	0.064	0.029
Remove	0.877	0.955	0.123	0.045
Move	0.937	0.982	0.063	0.018

Table 4.5: Sensitivity, Specificity, False Negative Rate, and False Positive Rate of Bond, Electron, Remove, and Move Sketches

5. DISCUSSION

This chapter discusses and interprets the results presented in the previous chapter. After reviewing the five categories of overall improvement, app molecule type improvement, non-app molecule scores, app interaction, and sketch recognition analysis, the chapter continues with presenting the current limitations of the study and future work.

5.1 Overall Improvement

The first question in the study addresses whether students that use the application with both paper-pencil techniques and immediate feedback experience a greater overall improvement in pre and post quiz scores. As table 4.4 and figure 4.5 show, both application versions caused an increase in quiz scores. While at first glance, the two versions seem to improve the quiz scores regardless of the application interaction, a further statistical analysis shows a difference between the two.

Table 4.1 presents the result of a Mann-Whitney U test and Two Sample T test when comparing score differences from both applications. For this sample size and significance level of 0.05, a critical value of U is determined to be 13. Comparing the pre-quiz and post-quiz scores resulted in a smaller U-value of 11 for the Paper-Pencil Techniques application, but not for the Undo Application, which had a U-value of 17. The Two Sample T test also resulted in a p-value of 0.0158 when comparing the score differences. Since the U-value of 11 is smaller than the critical U-value of 13, and the p-value of 0.0158 is less than the significance level of 0.05, both tests resulted in rejecting the null hypothesis for Paper-Pencil Techniques to claim that there is a significant difference between the score differences. The paper-pencil techniques had a higher score difference, and resulted in a higher average post-quiz score, so we can conclude that the application paper-pencil techniques experienced a greater overall improvement of quiz scores.

Since the overall improvement can be affected by the values given to each molecule when grading, an all-or-nothing grading method was also used to determine if the greater overall improvement still exists when the grade only depends on fully correct molecules. While figure 4.11

shows the paper-pencil techniques resulting in an overall greater improvement, a Mann-Whitney U test shows that the difference in improvement is not significant with this grading method.

5.2 App Molecule Type Improvement

To address the question on how the application versions differed in molecule type improvement, the scores are analyzed in three different categories for each molecule type. Using the post-quiz score results for individual molecules, figure 4.7 shows both the paper-pencil techniques application and undo application scoring well for single bonded molecules. Lower scores begin to appear for double bonded and triple bonded molecules. When comparing the applications, the undo application shows slightly more lower scores for multiple bonded molecules. Figure 4.8 also shows how the paper-pencil techniques application resulted in the quiz score difference to slowly surpass the undo application's quiz score difference as the molecules became more complex. When considering the all-or-nothing grading method, the molecule scores shown in figure 4.12 followed a similar pattern with the original grading method. However, a lower cut-off of 70% needed to be used to see this pattern, due to the overall lower scores when removing partial credit. When considering the question of how the application versions differed in molecule type improvement, these results allow us to infer that the paper-pencil techniques are contributing to a stronger performance for complex molecules regardless of whether partial credit is included or not.

5.3 Non-App Molecule Scores

Another question to address involves comparing the application's quiz performance for nonapp molecules. Figure 4.9 shows the post-quiz score results for non-app molecules with the paperpencil techniques application and the undo application. The undo application resulted in more low post-quiz scores compared to the paper-pencil techniques application. Only one molecule was not scored under 80% for the undo application, while the paper-pencil techniques application had three molecules that scored over 80%. The weighted all-or-nothing grading method resulted in an additional molecule flagged compared to the original grading method, however, figure 4.13 still shows more molecules scoring lower for this category. Non-App molecules show the participants performance when approaching new problems they have not seen the solution to. These types of molecules would require a stronger understanding of concepts than the remaining molecules on the quiz. When considering how the application versions compared to non-app molecules, the paper-pencil techniques performs better than the undo application, which suggests that the presence of the techniques are solidifying the concepts stronger than the undo application.

5.4 App Interaction

The final question to consider discusses whether there is any beneficial difference between the way students interact with the two application versions. A one tailed Mann-Whitney U test is used to compare the interactions shown in 4.14. With a significance level of 0.05 and a critical U value of 11, none of the smaller U values in 4.3 are below the critical U value. Therefore, we can not claim there is a significant difference between the way participants interacted with the application.

5.5 Sketch Recognition Analysis

The overall confusion matrix from table 4.4 is generated from a Leave One Out Cross Validation, where there is a total of 180 bonds, 360 electrons, 252 removes, and 126 moves. As the true positives show, most of the bonds, electrons, and moves were recognized correctly, with an accuracy of 97.2%, 93.6%, and 93.7% respectively. However, removes were recognized with the least accuracy of 87.7%. Additionally, table 4.5 shows that the remove gesture has the highest false negative rate of 12.3%. These results show that remove sketches weren't classified as correctly compared to the other gestures, and more sketches were incorrectly classified as a remove compared to other gestures. The difficulty in classifying the remove gesture can be explained due to the differences that occur for the gesture between participants. While drawing lines, small circles, and large circles is generally controlled and follows similar patters, the act of scribbling or scratching out has more freedom. Participants may choose to scratch out differently, as there aren't strict rules of how to scratch out. While the current sketch recognition features are still effective in identifying a remove, the freedom of scratching out can be analyzed more closely to help improve the accuracy of classifying remove gestures.

5.6 Limitations of the Study

Current limitations of the study that are discussed include sample size and pre-observation effects. When designing the study and analysis, these limitations have also been taken into consideration.

5.6.1 Sample Size and Generalizability

A total of 14 participants were recruited to the study where 7 used the application with paperpencil techniques and 7 used the undo application. Stronger results can be produced with increasing the sample size, however this sample size was taken into consideration during analysis by using a non-parametric statistical test. Additionally, participants were only recruited from undergraduate students with a basic chemistry background. Even though the sample size is smaller than desired, maintaining the target population during recruitment allows us to generalize the results to undergraduate students who do not have an advanced chemistry background.

5.6.2 Pre-Quiz Effects

Since an OX_1X_2O design is used for this study, it is common to bring up the effects of the first observation on the results. When all participants take a pre-quiz prior to the application, it becomes unknown of whether the pre-quiz itself causes the improvement in post-quiz scores rather than the application. While this question remains, the analysis of results is setup to compare the two applications. Since all participants have taken the same pre-quiz, that is remained as a control of the study. Both applications have caused some improvement in scores, but with the pre-quiz remaining as a control, we can infer that any difference in improvement are caused by the two applications.

5.7 Future Work

Future work for this study can involve a improvements in a variety of areas. These ideas are explained in the categories of application improvement and study setup changes.

5.7.1 Application Improvement

The current application is designed for basic molecules and introductory concepts. Design decisions include pre-arranging atoms, only including molecules with central atoms, limiting the number of atoms to 5, and not included advanced concepts and exceptions. While these decisions work for basic molecules, the application would need significant improvement for more complex molecules.

5.7.1.1 Sketch Recognition of Entire Molecule

The current application uses sketch recognition to interpret hand drawn bonds, electrons, and interaction techniques. The future application can incorporate identifying the entire chemical diagram, including the atoms. This would allow the entire sketchpad to act like paper with the freedom to draw anywhere. Techniques to recognize these components can be found in previous sketch recognition methods for chemical diagrams. [9].

5.7.1.2 Exceptions and Formal Charges

For this study, the Lewis dot diagram was deciphered in section 3.2.1 using only introductory concepts. The algorithms to check for the correct diagram follow the general rules for drawing molecules, however several complex molecules use exceptions to these general rules when formulating the correct diagram. A method for considering different exceptions would need to be created when checking advanced molecules. The concept of formal charges also needs to be considered when checking the arrangement of atoms and electrons.

5.7.2 Study Changes

Future work can also involve modifications to the study. This includes observing the effects of the application on different target populations, and using additional studies to help confirm and modify new paper-pencil techniques.

5.7.2.1 Target Population

The current study is set up to evaluate the performance of undergraduate students with basic chemistry knowledge. However, since the application is setup for introductory concepts, it would also be beneficial to assess how it performs for high school students who are taking a chemistry course for the first time. Learning to draw chemical diagrams can also be extended to organic chemistry with advanced chemical diagrams. Expanding the check algorithms to incorporate concepts from organic chemistry would be a long-term improvement in the future. This expansion can help the study infer how the application is beneficial for organic chemistry students.

5.7.2.2 Paper-Pencil Technique Identification

The current study uses previous research to identify which techniques to use in the application. A future study, however, could involve assessing the way students draw and edit Lewis dot diagrams, and identifying what interaction techniques they use on paper. Students can be asked to draw various molecules on paper, and their use of paper can be observed. The current paperpencil techniques can be confirmed, and new possible techniques can be identified. Additionally, the sketches that are used to perform the techniques can be observed.

6. CONCLUSION

In this study, two applications were created to investigate whether the integration of paperpencil techniques and immediate feedback results in a stronger ability to draw accurate Lewis Dot Diagrams compared to using an application without paper-pencil techniques. An analysis of prequiz scores, post-quiz scores, and application data creates a conclusion in the following categories.

- 1. **Overall Improvement** When comparing score differences between the two applications, participants who used the application with paper-pencil techniques experienced a greater improvement compared to participants who used the application with an undo button. The improvement between pre-quiz and post-quiz scores is greater for participants who only have a high school background of chemistry.
- 2. **Molecule Type Improvement** All participants struggled as molecules became more complex, however, participants who used the application with paper-pencil techniques scored higher on complex molecules.
- 3. **Non-App Molecule Improvement** Molecules that were not practiced on the application were the most difficult to solve on the post-quiz, however, participants who used the application with paper-pencil techniques scored higher than participants who used the application with an undo button.
- 4. **App Interaction Difference** When comparing the different interaction techniques saved from the application usage, there is no significant difference between the way participants interacted with each application. This suggests that the existence of paper-pencil techniques does not change the way participants use the immediate feedback.
- 5. **Sketch Recognition** The features determined by Rubine still continue to be effective in recognizing gestures with a decision tree classifier, however, modifying the application to recognize different scratch out gestures is necessary to improve classification.

The different types of improvement analysis suggest the paper-pencil techniques have an educational benefit for practicing Lewis dot diagrams, especially when the molecules are more complex. Since the application is more effective for participants with a high school background, there is motivation to expand the study to examine its effects in a high school setting. Additional improvements can be incorporated into the application to allow higher level chemistry students to practice advanced concepts, and further sketch recognition can be used to help identify the entire Lewis dot diagram drawing and interaction for the application.

REFERENCES

- A. C. Wilbraham, D. D. Staley, M. S. Matta, and E. L. Waterman, *Pearson Chemistry*. PRENTICE HALL, 2010.
- [2] J. M. Tiettmeyer, A. F. Coleman, R. S. Balok, T. W. Gampp, P. L. Duffy, K. M. Mazzarone, and N. P. Grove, "Unraveling the complexities: An investigation of the factors that induce load in chemistry students constructing lewis structures," *Journal of Chemical Education*, vol. 94, pp. 282–288, February 2017.
- [3] M. M. Cooper, N. Grove, S. M. Underwood, and M. W. Klymkowsky, "Lost in lewis structures: An investigation of student difficulties in developing representational competence," *Journal of Chemical Education*, vol. 87, no. 8, pp. 869–874, 2010.
- [4] P. Nassiff and W. A. Czerwinski, "Teaching beginning chemistry students simple lewis dot structures," *Journal of Chemical Education*, vol. 92, no. 8, pp. 1409–1411, 2015.
- [5] A. L. Kiste, R. G. Hooper, G. E. Scott, and S. D. Bush, "Atomic tiles: Manipulative resources for exploring bonding and molecular structure.," *Journal of Chemical Education*, vol. 93, no. 11, pp. 1900–1903, 2016.
- [6] M. S. Lewis, J. Zhao, and J. K. Montclare, "Development and implementation of high school chemistry modules using touch-screen technologies.," *Journal of Chemical Education*, vol. 89, no. 8, pp. 1012–1018, 2012.
- [7] R. Pargas, M. Cooper, C. Williams, and S. Bryfczynski, "Organicpad: A tablet pc based interactivity tool for organic chemistry.," *First International Workshop on Pen-Based Learning Technologies (PLT 20017)*, 2007.
- [8] O. Atilola, S. Valentine, H. Kim, D. Turner, E. Mctigue, T. Hammond, and J. Linsey, "Mechanix: A natural sketch interface tool for teaching truss analysis and free-body

diagrams.," Artificial Intelligence for Engineering Design, Analysis and Manufacturing, vol. 28, no. 2, pp. 169–192, 2014.

- [9] T. Y. Ouyang and R. Davis, "Chemink.," *Proceedings of the 15th International Conference* on Intelligent User Interfaces - IUI, vol. 11, 2011.
- [10] D. B. Smithrud and A. R. Pinhas, "PencilâĂŞpaper learning should be combined with online homework software.," *Journal of Chemical Education*, vol. 92, no. 12, pp. 1965–1970, 2015.
- [11] I. Kaufmann, K. M. Hamza, C. Rundgren, and L. Eriksson, "Developing an approach for teaching and learning about lewis structures," *International Journal of Science Education*, vol. 39, no. 12, pp. 1601–1624, 2017.
- [12] W.-Y. Ahmad and M. B. Zakaria, "Drawing lewis structures from lewis symbols: A direct electron-pairing appraoch.," *Journal of Chemical Education*, vol. 77, pp. 329–331, 2000.
- [13] J. A. Brady, J. N. Milbury-Steen, and J. L. Burmeister, "Lewis structure skills: Taxonomy and difficulty levels.," *Journal of Chemical Education*, vol. 67, pp. 491–493, 1990.
- [14] J. A. Carroll, "Drawing lewis structures without anticipating octets.," *Journal of Chemical Education*, vol. 63, pp. 28–31, 1986.
- [15] T. J. Clark, "Another procedure for writing lewis structures.," *Journal of Chemical Education*, vol. 61, p. 100, 1984.
- [16] R. L. Dekock, "The chemical bond.," *Journal of Chemical Education*, vol. 64, pp. 934–941, 1987.
- [17] D. Eberlin and M. Monroe, "A different approach to hybridization and geometric structure of simple molecules and ions.," *Journal of Chemical Education*, vol. 59, pp. 285–287, 1987.
- [18] K. Imkampe, "An alternative procedure for writing lewis structures.," *Journal of Chemical Education*, vol. 52, pp. 429–432, 1975.
- [19] A. B. P. Lever, "Lewis structures and the octet rule. an automatic procedure for writing canonical forms.," *Journal of Chemical Education*, vol. 49, pp. 819–821, 1972.

- [20] S. R. Logan, "The role of lewis structures in teaching covalent bonding.," *Journal of Chemical Education*, vol. 78, pp. 1457–1458, 2001.
- [21] C. J. Malerich, "Lewis structures for compounds with expanded octets.," *Journal of Chemi-cal Education*, vol. 64, p. 403, 1987.
- [22] E. C. McGoran, "Lone electron motion delocalization and relocalization to write lewis structures.," *Journal of Chemical Education*, vol. 68, pp. 19–23, 1991.
- [23] J. E. Packer and S. D. Woodgate, "Lewis structures, formal charge, and oxidation numbers: A more user-friendly approach.," *Journal of Chemical Education*, vol. 68, pp. 456–458, 1991.
- [24] J. Q. Pardo, "Teaching a model for writing lewis structures.," *Journal of Chemical Education*, vol. 66, pp. 456–458, 1989.
- [25] G. H. Purser, "Lewis structures are models for predicting molecular structure, not electronic structure.," *Journal of Chemical Education*, vol. 76, pp. 1013–1018, 1999.
- [26] G. H. Purser, "Lewis structures in general chemistry: Agreement between electron density calculations and lewis structures.," *Journal of Chemical Education*, vol. 78, pp. 981–983, 2001.
- [27] J. L. Reed, "The lewis structure: An expanded perspective.," *Journal of Chemical Education*, vol. 71, pp. 98–100, 1994.
- [28] L. Suidan, J. K. Badenhoop, E. D. Glendening, and F. Weinhold, "Common textbook and teaching misconceptions of lewis structures.," *Journal of Chemical Education*, vol. 72, pp. 583–586, 1995.
- [29] M. E. Zandler and E. R. Talaty, "The "6n + 2 rule" for writing lewis octet structures.," *Journal of Chemical Education*, vol. 61, pp. 124–127, 1984.

- [30] S. R. Singer, N. R. Nielsen, and H. A. Schweingruber, "Discipline-based education research: Understanding and improving learning in undergraduate science and engineering," *National Academies Press*, 2012.
- [31] S. Underwood, "Bridging the gap between structures and properties: An investigation and evaluation of studentsâĂŹ representational competence," *Ph.D. Dissertation, Clemson University*, 2011.
- [32] W. Breslyn, "Lewis structures: Considerations for teaching and learning," http://terpconnect.umd.edu/ wbreslyn/chemistry/Lewis- Structures/lewis-main.html, accessed October 2018.
- [33] W.-Y. Ahmad and O. Siraj, "Drawing lewis structures: A step-by- step approach," *Journal of Chemical Education*, vol. 69, no. 10, pp. 791–792, 1992.
- [34] K. B. T. S. Myers, R. T.; Oldham, "Holt chemistry," *Holt McDougal, New York*, pp. 200–206, 2006.
- [35] R. A. Burns, "Fundamentals of chemistry, 3rd ed," *Prentice Hall: Upper Saddle River, NJ*, pp. 233–238, 1999.
- [36] N. J. Tro, "Introductory chemistry essentials, 4th ed," *Prentice Hall, Upper Saddle River, NJ*, p. Chapter 10, 2011.
- [37] M. Antunes, M. A. R. Pacheco, and M. Giovanela, "Design and implementation of an educational game for teaching chemistry in higher education," *Journal of Chemical Education*, vol. 89, no. 4, pp. 517–521, 2012.
- [38] J. V. Russell, "Using games to teach chemistry: An annotated bibliography," *Journal of Chemical Education*, vol. 76, no. 4, pp. 481–484, 1999.
- [39] K. R. Ruddick and A. L. Parrill, "Ce classroom activity #113: An interlocking building block activity in writing formulas of ionic compounds," *Journal of Chemical Education*, vol. 89, no. 11, pp. 1436–1438, 2012.

- [40] R. Kozma and J. Russell, "Modelling students becoming chemists: Developing representational competence. in visualization in science education," *Gilbert, J. K., Ed.; Springer: Dordrecht*, pp. 121–145, 2005.
- [41] R. Kozma, "Material and social affordances of multiple representations for science understanding. in knowledge-in-the- making: Epistemological aspects of using inscriptions during teaching and learning science.," *Symposium Conducted at the Annual Meeting of the American Educational Research Association (AERA)*, 2001.
- [42] P. Schank and R. Kozma, "Learning chemistry through the use of a representation-based knowledge building environment," *J. Comput. Math. Sci. Teach.*, vol. 21, no. 3, pp. 253– 279, 2002.
- [43] R. Kozma, E. Chin, J. Russell, and N. Marx, "The roles of representations and tools in the chemistry laboratory and their implications for chemistry learning.," *J. Learn. Sci.*, vol. 9, no. 2, pp. 105–143, 2000.
- [44] M. Stieff, R. C. Bateman, Jr., and D. H. Uttal, "Teaching and learning with threedimensional representations. in visualization in science education," *Gilbert, J. K., Ed.; Springer: Dordrecht*, 2005.
- [45] B. B. Miburo, "Simplified lewis structure drawing for nonscience majors," *Journal of Chemical Education*, vol. 75, no. 3, p. 317, 1998.
- [46] M. Silberberg, "Chemistry: The molecular nature of matter and change," *Mosby: St. Louis, MO*, 1996.
- [47] L. N. Purdy, "The history of television & radio in continuing education.," New Directions for Adult and Continuing Education, vol. 5, pp. 15–29, 1980.
- [48] D. W. Brooks, "Technology in chemistry education," *Journal of Chemical Education*, vol. 70, pp. 705–707, 1993.
- [49] "http://schools.nyc.gov/studentsupport/default.html." Web, 2012.

- [50] "http://www.csulb.edu/ âĹijmurdock/histofcs.html." Web, 2012.
- [51] "http://education.jhu.edu/newhorizons/ education-technology-resources-1/index.html."Web, 2012.
- [52] K. J. Crippten and B. L. Earl, "Impact of web-based worked examples and self-explanation on performance, problem-solving, and self-efficacy.," *Computers and Education*, vol. 49, pp. 809–821, 2005.
- [53] O. McGarr, "A review of podcasting in higher education: Its influence on the traditional lecture.," *Australasian Journal of Education Technology*, vol. 25, no. 3, pp. 309–321, 2009.
- [54] S. Avramiotis and G. Tsaparlis, "Using computer simulations in chemistry problem solving.," *Chemistry Education Research and Practice.*, 2013.
- [55] R. Blonder, M. Jonatan, Z. Bar-Dov, N. Benny, S. Rap, and S. Sakhnini, "Can you tube it? providing chemistry teachers with technological tools and enhancing their self-efficacy beliefs.," *Chemistry Education Research and Practice.*, pp. 309–321, 2013.
- [56] R. C. Clarke and R. E. Mayer, "E-learning and the science of instruction," 2nd ed. San Francisco: Pfeiffer (Wiley), 2008.
- [57] Y. J. Dori and M. Barak, "A web-based chemistry course as a means to foster freshman learning.," *Journal of Chemical Education*, vol. 80, no. 9, pp. 1084–1092, 2003.
- [58] A. B. Flynn, "Developing problem-solving skills through retrosynthetic analysis and clickers in organic chemistry," *Journal of Chemical Education*, vol. 88, no. 11, pp. 1496–1500, 2011.
- [59] M. T. Gebru, A. J. Phelps, and G. Wulfsberg, "Effect of clickers versus online homework on students' long-term retention of general chemistry course material.," *Chemistry Education Research and Practice*, vol. 13, no. 3, pp. 325–329, 2012.
- [60] J. R. MacArthur and L. L. Jones, "A review of literature reports of clickers applicable to college chemistry classrooms.," *Chemistry Education Research and Practice*, vol. 9, pp. 187– 195, 2008.
- [61] D. Read and S. Lancaster, "Unlocking video: 24/7 learning for the ipod generation.," *Education in Chemistry*, vol. 49, no. 4, pp. 13–16, 2012.
- [62] D. P. Rosenthal and M. J. Sanger, "How does viewing one computer animation affect students' interpretations of another animation depicting the same oxidation-reduction reaction?," *Chemistry Education Research and Practice*, 2013.
- [63] B. J. Ryan, "Line up, line up: using technology to align and enhance peer learning and assessment in a student centered foundation organic chemistry module.," *Chemistry Education Research and Practice*, 2013.
- [64] M. K. Seery, "Moving an in-class module online: a case study for chemistry.," *Chemistry Education Research and Practice*, vol. 13, no. 1, pp. 39–46, 2012.
- [65] A. Inc, "Apple in education. mac, ipod, ipad and iphone for learning.," 2012. https://apple.com/education/why-apple/?kmed=ppc&gclid= CNLThNv76KgCFYfe4AoduGyGDg, 2012.
- [66] M. Koclğ, "Implications of learning theories for effective technology integration and preservice teacher training: A critical literature review," *Sci. Educ*, pp. 2–18, 2005.
- [67] S. Smith and I. Stovall, "Networked instructional chemistry using technology to teach chemistry," *Journal of Chemical Education*, vol. 73, pp. 911–915, 1996.
- [68] S. Banister, "Integrating the ipod touch in kâĹŠ12 education: Visions and vices," *Computers in the Schools 2010*, vol. 27, pp. 121–131, 2010.
- [69] S. Kessler, "8 ways technology is improving education," http:// mashable.com/2010/11/22/technology-in-education, accessed Dec 2018.
- [70] "cs.washington.edu/education/dl/presenter/ uw classroom presenter." Web.

- [71] "up.ucsd.edu/ ubiquitous presenter." Web.
- [72] R. Pargas, "Reducing lecture and increasing student activity in large computer science courses," Proc. 11th Annual Conf. on Innovation and Technology in Computer Science Education, Bologna, Italy, June 26-28, 2006.
- [73] J. Staff, "Comparison of features, electronic homework management systems," *Journal of Chemical Education*, vol. 86, p. 693, 2009.
- [74] L. L. Parker and G. M. Loudon, "G. m. case study using online homework in undergraduate organic chemistry: Results and student attitudes," *Journal of Chemical Education*, vol. 90, pp. 37–44, 2013.
- [75] J. Drelick, Z. Henry, M. Richards-Babb, and J. Robertson-Honecker, "Online homework, help or hindrance? what students think and how they perform.," *J. Coll. Sci. Teach*, vol. 40, pp. 81–93, 2011.
- [76] A. Mangen and J.-L. Velay, "Digitizing literacy: Reflections on the haptics of writing," *Advances in Haptics*, pp. 385–401, 2010.
- [77] M. Naka and H. Naoi, "The effect of repeated writing on memory.," *Memory & Cognition*, vol. 23, pp. 201–212, 1995.
- [78] C. Hulme, "The interaction of visual and motor memory for graphic forms following tracing.," *Quarterly Journal of Experimental Psychology*, vol. 31, pp. 249–261, 1979.
- [79] M. Longcamp, C. Boucard, J.-C. Gilhodes, and J.-L. Velay, "Remembering the orientation of newly learned characters depends on the associated writing knowledge: A comparison between handwriting and typing.," *Human Movement Science*, vol. 25, pp. 646–656, 2006.
- [80] H. Choi and T. Hammond, "Sketch recognition based on manifold learning," 23rd National Conference on Artificial Intelligence, vol. 3, pp. 1786–1787, 2008.
- [81] D. Rubine, "Specifying gestures by example.," Proceedings of the 18th annual conference on Computer graphics and interactive techniques, pp. 329–337, 1991.

- [82] R. Vatavu, L. Anthony, and J. Wobbrock, "Gestures as point clouds: a \$p recognizer for user interface prototypes," 14th ACM International Conference on Multimodal Interaction, pp. 273–280, 2012.
- [83] J. Wobbrock, A. Wilson, and Y. Li, "Gestures without libraries, toolkits or training: a \$1 recognizer for user interface prototypes.," 20th Annual ACM Symposium on User Interface Software and Technology, pp. 159–168, 2007.
- [84] T. Hammond and R. Davis, "Ladder, a sketching language for user interface developers.," *Compu. Graph*, vol. 4, no. 29, pp. 518–532, 2005.
- [85] B. Paulson and T. Hammond, "Paleosketch: accurate primitive sketch recognition and beautification.," 13th International Conference on Intelligent User Interfaces, pp. 1–10, 2008.
- [86] S. Belongie, J. Malik, and J. Puzicha, "Shape context: a new descriptor for shape matching and object recognition.," *NIPS*, vol. 2, p. 3, 2000.
- [87] L. Kara and T. Stahovich, "An image-based trainable symbol recognizer for sketch-based interfaces.," *AAAI Fall Symposium*, pp. 99–105, 2004.
- [88] E. Miller, N. Matsakis, P. Viola, and et al., "Learning from one example through shared densities on transforms.," *IEEE Conference on Computer Vision and Pattern Recognition*, vol. 1, pp. 464–471, 2000.
- [89] W. Rucklidge, "Efficient visual recognition using the hausdorff distance," *IEEE Conference* on Computer Vision and Pattern Recognition, p. 1996, 1173.
- [90] M. Prasad and T. Hammond, "Observational study on teaching artifacts created using tablet pc.," *CHI'12 Extended Abstracts on Human Factors in Computing Systems*, pp. 301–316, 2012.
- [91] O. Atilola, E. McTigue, T. Hammond, and J. Linsey, "Mechanix: evaluating the effectiveness of a sketch recognition truss tutoring program against other truss programs," *120th American Society for Engineering Education Annual Conference & Exposition*, vol. 15, 2013.

- [92] M. Field, S. Valentine, J. Linsey, and T. Hammond, "Sketch recognition algorithms for comparing complex and unpredictable shapes.," *Twenty-Second International Joint Conference on Artificial Intelligence*, vol. 3, pp. 2436–2441, 2011.
- [93] K. Kebodeaux, M. Field, and T. Hammond, "Defining precise measurements with sketched annotations," *Eighth Eurographics Symposium on Sketch-Based Interfaces and Modeling*, pp. 79–86, 2011.
- [94] S. Valentine, F. Vides, G. Lucchese, D. Turner, H. Kim, W. Li, J. Linsey, and T. Hammond, "Mechanix: a sketch-based tutoring and grading system for free-body diagrams.," *AI Mag.*, vol. 34, no. 1, p. 55, 2012.
- [95] S. Valentine, F. Vides, G. Lucchese, D. Turner, H. Kim, W. Li, J. Linsey, and T. Hammond, "Mechanix: a sketch-based tutoring system for statics courses," *IAAI*, 2012.
- [96] S. Ma, Y. Sun, P. Lyu, S. Polsley, and T. Hammond, "Dcsr: A digital circuit sketch recognition system for education," *Computers and Graphics*, pp. 137–146, 2017.
- [97] B. Edwards and V. Chandran, "Machine recognition of hand-drawn circuit diagrams," 2000 IEEE International Conference on Acoustics, Speech, and Signal Processing, vol. 6, pp. 3618–3621, 2000.
- [98] T. Sezgin and R. Davis, "Sketch recognition in interspersed drawings using time-based graphical models," *Compute. Graph.*, vol. 32, no. 5, pp. 500–510, 2008.
- [99] A. Niaz Bhat, G. Kasiviswanathan, C. Maria Mathew, S. Polsley, E. Prout, D. Goldberg, and T. Hammond, "An intelligent sketching interface for education using geographic information systems," *Frontiers in Pen and Touch*, pp. 147–163, 2017.
- [100] "https://terpconnect.umd.edu/ wbreslyn/chemistry/lewis-structures/lewis-main.html Lewis Structures." Web, 2012.

APPENDIX A

LEAVE ONE OUT CROSS VALIDATION DECISION TREES

Decision Trees from Leave One Out Cross Validation of each participants' training data collected in the tutorial page. The features from Rubine [81] are labeled in each decision tree as follows:

- Feature 1 cosineStartAngle cosine of the start angle
- Feature 2 sineStartAngle sine of the start angle
- Feature 3 BBDiagLen length of the bounding box diagonal
- Feature 4 BBDiagAngle angle of the bounding box
- Feature 5 startEndDist distance between start and endpoint
- Feature 6 startEndCosineAngle cosine of angle from start to endpoint
- Feature 7 startEndSineAngle sine of angle from start to endpoint
- Feature 8 strokeLength length of stroke
- Feature 9 angleTrav9 total angle
- Feature 10 angleTrav10 total absolute angle
- Feature 11 angleTrav11 sharpness
- Feature 12 maxSpeed maximum speed
- Feature 13 pathDuration time taken for entire stroke

```
J48 pruned tree
_____
BBDiagLen <= 19.416488
BBDiagLen <= 14.21267: electron (276.0/1.0)</p>
BBDiagLen > 14.21267
I I maxSpeed <= 0.055402: electron (26.0)</p>
| | maxSpeed > 0.055402
I I I strokeLength <= 40.633885: electron (21.0/1.0)</p>
| | | strokeLength > 40.633885
1 | | | angleTrav9 <= 6.823605: remove (8.0)</pre>
| | | | | angleTrav9 > 6.823605: electron (4.0)
BBDiagLen > 19.416488
I startEndDist <= 44.28318</pre>
I I startEndCosineAngle <= -0.6</p>
I I I BBDiagAngle <= 0.276097: remove (7.0)</p>
I I BBDiagAngle > 0.276097
| | | | BBDiagLen <= 30.479501: electron (3.0/1.0)
| | | | BBDiagLen > 30.479501
| | | | angleTrav9 <= 3.60524: remove (5.0/1.0)
| | | | | angleTrav9 > 3.60524
| | | | | | | angleTrav11 <= 10.253431: move (93.0)
| | | | | angleTrav11 > 10.253431
| | | | | | | | startEndCosineAngle <= -0.810679: move (6.0)
| | | | | | startEndCosineAngle > -0.810679: remove (4.0)
I I startEndCosineAngle > -0.6
I I I strokeLength <= 43.633885: electron (8.0/1.0)</p>
| | | strokeLength > 43.633885
I I I BBDiagLen <= 46.270941: remove (143.0)</p>
| | | | BBDiagLen > 46.270941
| | | | | pathDuration <= 399: move (5.0)
| | | | | pathDuration > 399: remove (25.0/2.0)
l startEndDist > 44.28318
1 | strokeLength <= 122.552041: bond (164.0)</pre>
| | strokeLength > 122.552041
I I BBDiagLen <= 84.593144: remove (25.0)</p>
| | | BBDiagLen > 84.593144
| | | | cosineStartAngle <= -0.980581: move (2.0)
| | | | cosineStartAngle > -0.980581: bond (3.0)
Number of Leaves :
                         19
Size of the tree :
                  37
```

Figure A.1: Leave One Out Cross Validation: Paper-Pencil Techniques Participant 1 Left Out in Training

```
J48 pruned tree
BBDiagLen <= 19.416488
I maxSpeed <= 0.052469: electron (253.0)</p>
I maxSpeed > 0.052469
I I strokeLength <= 40.633885: electron (65.0/2.0)</p>
I I strokeLength > 40.633885
1 | angleTrav9 <= 5.961435: remove (9.0/1.0)</pre>
I I angleTrav9 > 5.961435: electron (8.0)
BBDiagLen > 19.416488
startEndDist <= 56.435804</pre>
I startEndCosineAngle <= -0.447214</p>
| | | BBDiagLen <= 39.698866
I I I I BBDiagLen <= 24.186773: electron (2.0)
| | | | BBDiagLen > 24.186773: remove (3.0)
I I I BBDiagLen > 39.698866
I I I BBDiagAngle <= 0.29473: remove (10.0/1.0)</p>
I I I BBDiagAngle > 0.29473
| | | | | strokeLength <= 308.187476: move (104.0/2.0)
| | | | | strokeLength > 308.187476: remove (3.0)
I l startEndCosineAngle > -0.447214
| | | strokeLength <= 43.633885: electron (7.0)
| | | strokeLength > 43.633885
| | | | BBDiagAngle <= 1.401018
| | | | | startEndDist <= 6.708204
| | | | | angleTrav9 <= 5.176037: remove (9.0)
| | | | | | | angleTrav9 > 5.176037: move (4.0)
| | | | | startEndDist > 6.708204: remove (161.0/1.0)
| | | | BBDiagAngle > 1.401018
| | | | | | BBDiagLen \le 56.035703: bond (4.0/1.0)
| | | | | BBDiagLen > 56.035703: remove (5.0)
startEndDist > 56.435804
I I strokeLength <= 122.552041: bond (161.0)</pre>
I I strokeLength > 122.552041
I I BBDiagLen <= 127.632284: remove (16.0)</p>
| | | BBDiagLen > 127.632284: bond (4.0/1.0)
Number of Leaves :
                         18
Size of the tree :
                  35
```

Figure A.2: Leave One Out Cross Validation: Paper-Pencil Techniques Participant 2 Left Out in Training

J48 pruned tree ------BBDiagLen <= 19.416488 I maxSpeed <= 0.052469: electron (252.0)</p> I maxSpeed > 0.052469 I I strokeLength <= 40.633885: electron (66.0/2.0) strokeLength > 40.633885 1 | angleTrav9 <= 6.038207: remove (9.0/1.0)</pre> | | | angleTrav9 > 6.038207: electron (8.0) BBDiagLen > 19.416488 I startEndDist <= 54.230987</p> I I startEndCosineAngle <= -0.6</p> | | | angleTrav11 <= 7.704851: move (88.0/1.0) | | | angleTrav11 > 7.704851 | | | | BBDiagLen <= 80.099938 | | | | BBDiagLen <= 24.186773: electron (2.0) | | | | BBDiagLen > 24.186773: remove (13.0/1.0) I I I BBDiagLen > 80.099938: move (14.0) I I startEndCosineAngle > -0.6 | | | pathDuration <= 256 | | | | angleTrav9 <= -0.785398: electron (6.0) | | | | | angleTrav9 > -0.785398: bond (4.0/1.0) | | | pathDuration > 256 | | | | maxSpeed <= 0.086505 | | | | BBDiagLen <= 35.510562: remove (4.0) BBDiagLen > 35.510562 | | | | | | | cosineStartAngle <= -0.090536: bond (2.0)| | | | | | | cosineStartAngle > -0.090536: electron (2.0) | | | | maxSpeed > 0.086505 | | | | angleTrav11 <= 4.993609 | | | | | angleTrav9 <= 5.092895: remove (24.0) | | | | | angleTrav9 > 5.092895: move (5.0) | | | | | angleTrav11 > 4.993609: remove (148.0) I startEndDist > 54.230987 I strokeLength <= 122.552041: bond (160.0)</p> strokeLength > 122.552041 | | | BBDiagLen <= 127.632284: remove (17.0) I I BBDiagLen > 127.632284: bond (4.0/1.0) Number of Leaves : 19 Size of the tree : 37

Figure A.3: Leave One Out Cross Validation: Paper-Pencil Techniques Participant 3 Left Out in Training

```
_____
BBDiagLen <= 20.615528
BBDiagLen <= 17.204651: electron (320.0/1.0)
| BBDiagLen > 17.204651
I startEndCosineAngle <= 0.496139: electron (8.0)</p>
I I startEndCosineAngle > 0.496139
| | | strokeLength <= 52.14433: electron (4.0/1.0)
1 | strokeLength > 52.14433: remove (5.0)
BBDiagLen > 20.615528
I startEndDist <= 56.435804</p>
I I startEndCosineAngle <= -0.694595</pre>
I I I BBDiagAngle <= 0.276097: remove (7.0)</p>
I I BBDiagAngle > 0.276097
| | | | angleTrav9 <= 3.60524
| | | | | cosineStartAngle <= -0.847998: remove (3.0)
| | | | | cosineStartAngle > -0.847998: electron (2.0/1.0)
| | | | angleTrav9 > 3.60524
| | | | angleTrav9 <= 9.888426: move (103.0/1.0)
| | | | angleTrav9 > 9.888426: remove (3.0/1.0)
I I startEndCosineAngle > -0.694595
I I I strokeLength <= 54.171205</p>
 | | | angleTrav9 <= -0.785398: electron (5.0)
L
| | | | angleTrav9 > -0.785398: bond (5.0)
| | | strokeLength > 54.171205
| | | | angleTrav11 <= 4.81265
| | | | angleTrav9 <= 5.03414: remove (21.0/1.0)
| | | | | | angleTrav9 > 5.03414: move (3.0)
| | | | angleTrav11 > 4.81265: remove (157.0)
I startEndDist > 56.435804
I strokeLength <= 117.124133: bond (159.0)</p>
| | strokeLength > 117.124133
      BBDiagLen <= 122.118795: remove (19.0)
I I BBDiagLen > 122.118795: bond (4.0/1.0)
Number of Leaves :
                         17
Size of the tree :
                  33
```

Figure A.4: Leave One Out Cross Validation: Paper-Pencil Techniques Participant 4 Left Out in Training

BBDiagLen <= 19.416488 1 maxSpeed <= 0.052469: electron (253.0)</pre> I maxSpeed > 0.052469 I I strokeLength <= 40.633885: electron (65.0/2.0)</pre> I strokeLength > 40.633885 1 | angleTrav9 <= 6.038207: remove (9.0/1.0)</pre> | | | angleTrav9 > 6.038207: electron (8.0) BBDiagLen > 19.416488 I startEndDist <= 56.435804</pre> | | startEndCosineAngle <= -0.447214 | | | angleTrav9 <= 5.092895 | | | | | maxSpeed <= 0.578125: move (7.0)| | | | | maxSpeed > 0.578125: remove (10.0/1.0) | | | angleTrav9 > 5.092895 | | | angleTrav11 <= 9.58703: move (92.0) | | | | angleTrav11 > 9.58703 | | | | | pathDuration <= 914: remove (4.0/1.0) | | | | | pathDuration > 914: move (5.0) I l startEndCosineAngle > -0.447214 | | | pathDuration <= 256 | | | | angleTrav9 <= -0.785398: electron (6.0) | | | | angleTrav9 > -0.785398: bond (5.0/1.0) | | | pathDuration > 256 | | | | maxSpeed <= 0.086505 | | | | BBDiagLen <= 35.510562: remove (4.0) | | | | | BBDiagLen > 35.510562 | | | | | | | cosineStartAngle <= -0.090536: bond (2.0)| | | | | | | cosineStartAngle > -0.090536: electron (2.0) | | | | maxSpeed > 0.086505 | | | | | startEndDist <= 6.708204 | | | | | angleTrav9 <= 5.176037: remove (11.0) | | | | | angleTrav9 > 5.176037: move (4.0) | | | | | startEndDist > 6.708204: remove (164.0) l startEndDist > 56.435804 I I strokeLength <= 122.552041: bond (159.0)</pre> | | strokeLength > 122.552041 | | | BBDiagLen <= 127.632284: remove (15.0) | | | BBDiagLen > 127.632284: bond (3.0) Number of Leaves : 20 Size of the tree : 39



```
J48 pruned tree
```

Size of the tree :

```
BBDiagLen <= 20.615528: electron (334.0/7.0)
BBDiagLen > 20.615528
l startEndDist <= 56.435804</pre>
I I startEndCosineAngle <= -0.6</p>
I I I strokeLength <= 308.187476</pre>
| | | | | angleTrav11 <= 7.832142: move (92.0)
| | | | angleTrav11 > 7.832142
| | | | BBDiagLen <= 79.40403: remove (8.0/2.0)
| | | | | BBDiagLen > 79.40403: move (9.0)
I I I strokeLength > 308.187476: remove (7.0)
I I startEndCosineAngle > -0.6
| | | pathDuration <= 256
I I I angleTrav9 <= -0.785398: electron (5.0)</p>
| | | | angleTrav9 > -0.785398: bond (5.0/1.0)
| | | pathDuration > 256
| | | | maxSpeed <= 0.09
| | | | | | cosineStartAngle <= -0.478852: remove (2.0)
| | | | | cosineStartAngle > -0.478852
| | | | | | | cosineStartAngle <= -0.099504: bond (2.0)
| | | | | | cosineStartAngle > -0.099504: electron (2.0)
| | | | maxSpeed > 0.09
| | | | pathDuration <= 333
| | | | | angleTrav9 <= 6.08579: remove (10.0)
| | | | | angleTrav9 > 6.08579: move (4.0)
| | | | | | | pathDuration > 333: remove (170.0/1.0)
startEndDist > 56.435804
1 l strokeLength <= 134.246985: bond (160.0)</pre>
I l strokeLength > 134.246985
I I I BBDiagLen <= 127.632284: remove (15.0)</p>
I I BBDiagLen > 127.632284: bond (3.0/1.0)
Number of Leaves :
                         16
```

Figure A.6: Leave One Out Cross Validation: Paper-Pencil Techniques Participant 6 Left Out in Training

31

```
J48 pruned tree
BBDiagLen <= 19.416488
I maxSpeed <= 0.052469: electron (268.0)</p>
I maxSpeed > 0.052469
I BBDiagLen <= 17.204651: electron (67.0/5.0)</p>
I BBDiagLen > 17.204651: remove (6.0/1.0)
BBDiagLen > 19.416488
1 startEndDist <= 56.435804</pre>
I l startEndCosineAngle <= -0.707107</pre>
I I BBDiagLen <= 30.479501: electron (3.0/1.0)</p>
I I BBDiagLen > 30.479501
I I I BBDiagAngle <= 0.3274
| | | | BBDiagLen <= 78.638413: remove (8.0)
| | | | BBDiagLen > 78.638413: move (7.0)
I I I BBDiagAngle > 0.3274: move (94.0/1.0)
I startEndCosineAngle > -0.707107
| | | BBDiagAngle <= 1.373401
I I I BBDiagLen <= 52.40229: remove (146.0)</p>
| | | | BBDiagLen > 52.40229
1 | | | strokeLength <= 162.691209: move (6.0)</pre>
| | | | strokeLength > 162.691209: remove (27.0/1.0)
I I BBDiagAngle > 1.373401
| | | | BBDiagLen <= 56.035703
| | | | BBDiagAngle <= 1.436475: electron (2.0)
| | | | BBDiagAngle > 1.436475: bond (4.0)
| | | | BBDiagLen > 56.035703: remove (7.0)
l startEndDist > 56.435804
1 strokeLength <= 122.552041: bond (161.0)</pre>
I l strokeLength > 122.552041
I I BBDiagLen <= 127.632284: remove (18.0)</p>
I I BBDiagLen > 127.632284: bond (4.0/1.0)
Number of Leaves :
                        16
Size of the tree :
                  31
```

Figure A.7: Leave One Out Cross Validation: Paper-Pencil Techniques Participant 7 Left Out in Training

```
BBDiagLen <= 19.416488
l maxSpeed <= 0.052469: electron (264.0)</pre>
l maxSpeed > 0.052469
1 | strokeLength <= 40.633885: electron (54.0/2.0)</pre>
1 | strokeLength > 40.633885
1 | angleTrav9 <= 6.038207: remove (9.0/1.0)</pre>
| | | angleTrav9 > 6.038207: electron (8.0)
BBDiagLen > 19.416488
startEndDist <= 56.435804
| | startEndCosineAngle <= -0.6
I I BBDiagAngle <= 0.276097: remove (7.0)</p>
| | | BBDiagAngle > 0.276097
| | | | angleTrav9 <= 3.60524
| | | | | cosineStartAngle <= -0.808736: remove (4.0)</p>
I I I I CosineStartAngle > -0.808736: electron (2.0/1.0)
| | | angleTrav9 > 3.60524
| | | | angleTrav11 <= 9.58703: move (110.0)
| | | | | angleTrav11 > 9.58703
I I I I I StartEndCosineAngle <= -0.824042: move (8.0)</p>
| | | | | | startEndCosineAngle > -0.824042: remove (6.0/1.0)
| | startEndCosineAngle > -0.6
| | | pathDuration <= 256
| | | | angleTrav9 <= -0.785398: electron (6.0)</p>
| | | | angleTrav9 > -0.785398: bond (5.0/1.0)
| | | pathDuration > 256
| | | | maxSpeed <= 0.086505
| | | | BBDiagLen <= 35.510562: remove (4.0)
| | | | BBDiagLen > 35.510562
| | | | | | cosineStartAngle <= -0.090536: bond (2.0)
| | | | | | | cosineStartAngle > -0.090536: electron (2.0)
| | | | maxSpeed > 0.086505
| | | | angleTrav11 <= 4.993609
| | | | | angleTrav9 <= 5.092895: remove (29.0)
| | | | | angleTrav9 > 5.092895: move (6.0)
| | | | angleTrav11 > 4.993609: remove (174.0)
I startEndDist > 56.435804
I I strokeLength <= 122.552041: bond (159.0)</pre>
I strokeLength > 122.552041
I I BBDiagLen <= 127.632284: remove (19.0)</p>
| | | BBDiagLen > 127.632284: bond (4.0/1.0)
Number of Leaves :
                         21
Size of the tree :
                  41
```

Figure A.8: Leave One Out Cross Validation: Undo Participant 1 Left Out in Training

```
BBDiagLen <= 19.416488
strokeLength <= 40.633885: electron (298.0/2.0)</pre>
l strokeLength > 40.633885
| | pathDuration <= 441
| | | maxSpeed <= 0.052469: electron (3.0)
| | | maxSpeed > 0.052469: remove (8.0)
1 | pathDuration > 441: electron (26.0)
BBDiagLen > 19.416488
I startEndDist <= 56.435804</p>
I I startEndCosineAngle <= -0.6</pre>
I I BBDiagAngle <= 0.276097: remove (7.0)</p>
| | | BBDiagAngle > 0.276097
| | | | angleTrav9 <= 3.60524
| | | | | | cosineStartAngle <= -0.808736: remove (4.0)
| | | | | cosineStartAngle > -0.808736: electron (2.0/1.0)
| | | | angleTrav9 > 3.60524
| | | | angleTrav11 <= 9.58703: move (110.0)
| | | | | angleTrav11 > 9.58703
1 | | | | startEndCosineAngle <= -0.824042: move (8.0)</pre>
1 | | | | startEndCosineAngle > -0.824042: remove (6.0/1.0)
I startEndCosineAngle > -0.6
| | | pathDuration <= 256
| | | | angleTrav9 <= -0.785398: electron (6.0)
| | | | angleTrav9 > -0.785398: bond (5.0/1.0)
| | | pathDuration > 256
| | | | maxSpeed <= 0.086505
| | | | BBDiagLen <= 35.510562: remove (4.0)
| | | | BBDiagLen > 35.510562
| | | | | cosineStartAngle <= -0.090536: bond (2.0)</pre>
I I I I I I cosineStartAngle > -0.090536: electron (2.0)
| | | | maxSpeed > 0.086505
| | | | angleTrav11 <= 4.993609
| | | | | angleTrav9 <= 5.092895: remove (29.0)
| | | | | angleTrav9 > 5.092895: move (6.0)
| | | | angleTrav11 > 4.993609: remove (174.0)
startEndDist > 56.435804
1 strokeLength <= 122.552041: bond (160.0)</pre>
| | strokeLength > 122.552041
I I BBDiagLen <= 127.632284: remove (19.0)</p>
I I BBDiagLen > 127.632284: bond (3.0/1.0)
Number of Leaves :
                        21
Size of the tree :
                  41
```

Figure A.9: Leave One Out Cross Validation: Undo Participant 2 Left Out in Training

```
BBDiagLen <= 19.416488
1 maxSpeed <= 0.052469: electron (255.0)</pre>
I maxSpeed > 0.052469
I strokeLength <= 40.633885: electron (63.0/2.0)</p>
I I strokeLength > 40.633885
1 | angleTrav9 <= 6.038207: remove (9.0/1.0)</pre>
| | | angleTrav9 > 6.038207: electron (8.0)
BBDiagLen > 19.416488
startEndDist <= 56.435804</pre>
I I startEndCosineAngle <= -0.6</p>
I I BBDiagAngle <= 0.276097: remove (7.0)</p>
I I BBDiagAngle > 0.276097
| | | | angleTrav9 <= 3.60524
| | | | | | cosineStartAngle <= -0.808736: remove (4.0)
| | | | | cosineStartAngle > -0.808736: electron (2.0/1.0)
| | | | angleTrav9 > 3.60524
| | | | angleTrav11 <= 9.58703: move (110.0)
| | | | | angleTrav11 > 9.58703
| | | | | startEndCosineAngle <= -0.824042: move (8.0)</pre>
| | | | | startEndCosineAngle > -0.824042: remove (6.0/1.0)
I I startEndCosineAngle > -0.6
| | | pathDuration <= 256
| | | | angleTrav9 <= -0.785398: electron (6.0)
| | | | angleTrav9 > -0.785398: bond (5.0/1.0)
| | | pathDuration > 256
| | | | maxSpeed <= 0.086505
| | | | BBDiagLen <= 35.510562: remove (4.0)
| | | | BBDiagLen > 35.510562
| | | | | cosineStartAngle <= -0.090536: bond (2.0)</pre>
I I I I I I cosineStartAngle > -0.090536: electron (2.0)
| | | | maxSpeed > 0.086505
| | | | angleTrav11 <= 4.993609
1 | | | | angleTrav9 <= 5.092895: remove (29.0)</pre>
| | | | | angleTrav9 > 5.092895: move (6.0)
| | | | angleTrav11 > 4.993609: remove (174.0)
startEndDist > 56.435804
1 | strokeLength <= 122.552041: bond (159.0)</pre>
| | strokeLength > 122.552041
| | | BBDiagLen <= 127.632284: remove (19.0)
I I BBDiagLen > 127.632284: bond (4.0/1.0)
Number of Leaves :
                         21
Size of the tree :
                  41
```

Figure A.10: Leave One Out Cross Validation: Undo Participant 3 Left Out in Training

```
BBDiagLen <= 19.416488
I maxSpeed <= 0.052469: electron (261.0)</p>
I maxSpeed > 0.052469
I I strokeLength <= 40.633885</pre>
| | | maxSpeed <= 0.057778
1 | | | cosineStartAngle <= -0.4741: remove (2.0)</pre>
| | | | cosineStartAngle > -0.4741: electron (6.0)
| | | maxSpeed > 0.057778: electron (49.0)
I I strokeLength > 40.633885
1 | angleTrav9 <= 6.038207: remove (9.0/1.0)</pre>
| | | angleTrav9 > 6.038207: electron (8.0)
BBDiagLen > 19.416488
l startEndDist <= 57.078893</pre>
I I startEndCosineAngle <= -0.6</pre>
I I BBDiagAngle <= 0.276097: remove (7.0)</p>
I I BBDiagAngle > 0.276097
| | | | angleTrav9 <= 3.60524
| | | | | cosineStartAngle <= -0.808736: remove (4.0)</p>
| | | | | cosineStartAngle > -0.808736: electron (2.0/1.0)
| | | | angleTrav9 > 3.60524
| | | | angleTrav11 <= 9.58703: move (110.0)
| | | | angleTrav11 > 9.58703
| | | | | startEndCosineAngle <= -0.824042: move (8.0)</p>
| | | | | startEndCosineAngle > -0.824042: remove (6.0/1.0)
I I startEndCosineAngle > -0.6
1 | strokeLength <= 48.950316</pre>
I I I I strokeLength <= 43.633885: electron (8.0/1.0)</p>
| | | | strokeLength > 43.633885
| | | | BBDiagLen <= 35.341194: remove (2.0)
| | | | BBDiagLen > 35.341194: bond (2.0)
I I strokeLength > 48.950316
| | | | angleTrav11 <= 4.993609
| | | | angleTrav9 <= 5.092895: remove (30.0/1.0)
| | | | angleTrav9 > 5.092895: move (6.0)
| | | | angleTrav11 > 4.993609: remove (179.0/1.0)
startEndDist > 57.078893
1 | strokeLength <= 122.552041: bond (161.0)</pre>
I strokeLength > 122.552041
I I BBDiagLen <= 127.632284: remove (18.0)</p>
| | | BBDiagLen > 127.632284: bond (4.0/1.0)
Number of Leaves :
                         21
Size of the tree :
                  41
```

Figure A.11: Leave One Out Cross Validation: Undo Participant 4 Left Out in Training

```
J48 pruned tree
```

```
BBDiagLen <= 19.416488
BBDiagLen <= 14.21267: electron (285.0/1.0)
BBDiagLen > 14.21267
I strokeLength <= 40.633885: electron (30.0/1.0)</p>
I I strokeLength > 40.633885
1 | angleTrav9 <= 6.283185: remove (9.0/1.0)</pre>
| | | angleTrav9 > 6.283185: electron (11.0)
BBDiagLen > 19.416488
startEndDist <= 56.435804</pre>
I I startEndCosineAngle <= -0.6</pre>
I I BBDiagAngle <= 0.276097: remove (7.0)</p>
I I BBDiagAngle > 0.276097
| | | | angleTrav9 <= 3.60524
| | | | | cosineStartAngle <= -0.808736: remove (4.0)</p>
| | | | | cosineStartAngle > -0.808736: electron (2.0/1.0)
| | | | angleTrav9 > 3.60524
| | | | angleTrav11 <= 9.58703: move (110.0)</pre>
| | | | | angleTrav11 > 9.58703
| | | | | | startEndCosineAngle <= -0.824042: move (8.0)
I I I I I StartEndCosineAngle > -0.824042: remove (6.0/1.0)
I I startEndCosineAngle > -0.6
| | | pathDuration <= 256
| | | | angleTrav9 <= -0.785398: electron (6.0)
| | | | angleTrav9 > -0.785398: bond (5.0/1.0)
I I I pathDuration > 256
| | | | maxSpeed <= 0.086505
| | | | BBDiagLen <= 35.510562: remove (4.0)
| | | | | BBDiagLen > 35.510562
| | | | | | | cosineStartAngle <= -0.090536: bond (2.0)
| | | | | cosineStartAngle > -0.090536: electron (2.0)
| | | | maxSpeed > 0.086505
| | | | | angleTrav11 <= 4.993609
| | | | | angleTrav9 <= 5.092895: remove (29.0)
| | | | | angleTrav9 > 5.092895: move (6.0)
| | | | angleTrav11 > 4.993609: remove (174.0)
startEndDist > 56.435804
I I strokeLength <= 122.552041: bond (159.0)</pre>
I strokeLength > 122.552041
BBDiagLen <= 127.632284: remove (19.0)
| | | BBDiagLen > 127.632284: bond (4.0/1.0)
Number of Leaves :
                         21
Size of the tree :
                  41
```

Figure A.12: Leave One Out Cross Validation: Undo Participant 5 Left Out in Training

```
BBDiagLen <= 19.416488
1 maxSpeed <= 0.052469: electron (258.0)</pre>
| maxSpeed > 0.052469
1 | strokeLength <= 40.633885: electron (60.0/2.0)</pre>
1 | strokeLength > 40.633885
1 | angleTrav9 <= 6.038207: remove (9.0/1.0)</pre>
| | | angleTrav9 > 6.038207: electron (8.0)
BBDiagLen > 19.416488
startEndDist <= 56.435804</pre>
I I startEndCosineAngle <= -0.6</p>
I I BBDiagAngle <= 0.276097: remove (7.0)</p>
| | | BBDiagAngle > 0.276097
| | | | angleTrav9 <= 3.60524
| | | | | cosineStartAngle <= -0.808736: remove (4.0)</p>
| | | | | cosineStartAngle > -0.808736: electron (2.0/1.0)
| | | | angleTrav9 > 3.60524
| | | | angleTrav11 <= 9.58703: move (110.0)
| | | | | angleTrav11 > 9.58703
| | | | | | | startEndCosineAngle <= -0.824042: move (8.0)
| | | | | | startEndCosineAngle > -0.824042: remove (6.0/1.0)
| | startEndCosineAngle > -0.6
| | | pathDuration <= 256
| | | angleTrav9 <= -0.785398: electron (6.0)</pre>
| | | | angleTrav9 > -0.785398: bond (5.0/1.0)
| | | pathDuration > 256
| | | | maxSpeed <= 0.086505
| | | | BBDiagLen <= 35.510562: remove (4.0)
| | | | BBDiagLen > 35.510562
| | | | | | cosineStartAngle <= -0.090536: bond (2.0)
| | | | | | | cosineStartAngle > -0.090536: electron (2.0)
| | | | maxSpeed > 0.086505
| | | | angleTrav11 <= 4.993609
| | | | | angleTrav9 <= 5.092895: remove (29.0)
| | | | | angleTrav9 > 5.092895: move (6.0)
| | | | angleTrav11 > 4.993609: remove (174.0)
startEndDist > 56.435804
I I strokeLength <= 122.552041: bond (159.0)</pre>
| | strokeLength > 122.552041
I I BBDiagLen <= 127.632284: remove (19.0)</p>
| | | BBDiagLen > 127.632284: bond (4.0/1.0)
Number of Leaves :
                         21
Size of the tree :
                  41
```

Figure A.13: Leave One Out Cross Validation: Undo Participant 6 Left Out in Training

```
J48 pruned tree
BBDiagLen <= 19.416488
1 maxSpeed <= 0.052469: electron (255.0)</pre>
I maxSpeed > 0.052469
I strokeLength <= 40.601126: electron (63.0/2.0)</p>
1 strokeLength > 40.601126
1 | angleTrav9 <= 6.038207: remove (9.0/1.0)</pre>
| | | angleTrav9 > 6.038207: electron (8.0)
BBDiagLen > 19.416488
startEndDist <= 56.435804</pre>
I l startEndCosineAngle <= -0.6</pre>
I I BBDiagAngle <= 0.276097: remove (7.0)</p>
I I BBDiagAngle > 0.276097
| | | | angleTrav9 <= 3.60524
| | | | | cosineStartAngle <= -0.808736: remove (4.0)</p>
| | | | | cosineStartAngle > -0.808736: electron (2.0/1.0)
| | | | angleTrav9 > 3.60524
| | | | angleTrav11 <= 9.58703: move (110.0)
| | | | angleTrav11 > 9.58703
| | | | | startEndCosineAngle <= -0.824042: move (8.0)</p>
1 | | | | startEndCosineAngle > -0.824042: remove (6.0/1.0)
I I startEndCosineAngle > -0.6
| | | pathDuration <= 256
| | | | angleTrav9 <= -0.785398: electron (6.0)
| | | | angleTrav9 > -0.785398: bond (5.0/1.0)
| | | pathDuration > 256
| | | | maxSpeed <= 0.086505
| | | | BBDiagLen <= 35.510562: remove (4.0)
| | | | BBDiagLen > 35.510562
| | | | | | | cosineStartAngle <= -0.090536: bond (2.0)
| | | | | | | cosineStartAngle > -0.090536: electron (2.0)
| | | | maxSpeed > 0.086505
| | | | angleTrav11 <= 4.993609
| | | | | angleTrav9 <= 5.092895: remove (29.0)
| | | | | angleTrav9 > 5.092895: move (6.0)
| | | | angleTrav11 > 4.993609: remove (174.0)
startEndDist > 56.435804
1 strokeLength <= 122.552041: bond (160.0)</pre>
1 strokeLength > 122.552041
I I BBDiagLen <= 127.632284: remove (19.0)</p>
| | | BBDiagLen > 127.632284: bond (3.0/1.0)
Number of Leaves :
                         21
Size of the tree :
                  41
```

Figure A.14: Leave One Out Cross Validation: Undo Participant 7 Left Out in Training

```
J48 pruned tree
  _____
BBDiagLen <= 19.209373
 strokeLength <= 41.306608: electron (307.0/2.0)
L
strokeLength > 41.306608
1 | maxSpeed <= 0.059172: electron (20.0)</pre>
| | maxSpeed > 0.059172
| | | angleTrav9 <= 6.038207: remove (8.0)
| | | angleTrav9 > 6.038207: electron (2.0)
BBDiagLen > 19.209373
  startEndDist <= 56.435804
L
I I startEndCosineAngle <= -0.6</p>
I I BBDiagAngle <= 0.276097: remove (7.0)</p>
I I BBDiagAngle > 0.276097
| | | | angleTrav9 <= 3.60524: remove (5.0/1.0)
| | | | angleTrav9 > 3.60524
| | | | angleTrav11 <= 10.253431: move (111.0)
  | | | angleTrav11 > 10.253431
| | | | | | startEndCosineAngle <= -0.824042: move (7.0)</p>
| | | | | | startEndCosineAngle > -0.824042: remove (5.0)
I l startEndCosineAngle > -0.6
| | | pathDuration <= 256
| | | | angleTrav9 <= -0.785398: electron (6.0)</p>
| | | | angleTrav9 > -0.785398: bond (5.0/1.0)
| | | pathDuration > 256
  | | | maxSpeed <= 0.086505
| | | BBDiagLen <= 35.510562: remove (4.0)
BBDiagLen > 35.510562
| | | | | | cosineStartAngle <= -0.090536: bond (2.0)</p>
| | | | | | | cosineStartAngle > -0.090536: electron (2.0)
| | | | maxSpeed > 0.086505
| | | | angleTrav11 <= 4.993609
| | | | | angleTrav9 <= 5.092895: remove (29.0)
| | | | | angleTrav9 > 5.092895: move (6.0)
| | | | angleTrav11 > 4.993609: remove (174.0)
startEndDist > 56.435804
    strokeLength <= 122.552041: bond (159.0)
| | strokeLength > 122.552041
I I BBDiagLen <= 127.632284: remove (19.0)</p>
| | | BBDiagLen > 127.632284: bond (4.0/1.0)
Number of Leaves :
                        20
Size of the tree :
                  39
```

Figure A.15: Leave One Out Cross Validation: Undo Participant 8 Left Out in Training