Revised Report on Generating Phase Diagram Graphs for Chemical Analysis

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Introduction:

Phase diagrams are an essential tool in chemical analysis and research, providing a visual representation of the relationship between temperature, pressure, and composition of different chemical compounds. Generating phase diagrams can be a challenging and time-consuming process, requiring extensive research and experimentation. In this report, we explain our progress and show how we have explored different methods of generating phase diagrams using innovative techniques such as data augmentation, neural networks, and OpenCV. This project idea was introduced to us by our lecturer Simona Orzan, where two groups are assigned on this project to get the results needed.

Data Collection:

As a group of two, we have looked to collect data from various sources. However, we have recently obtained input and output data from our main stakeholder consisting of 7 input graphs and 7 output graphs. Our aim is to increase the amount of input data to train our neural network models and generate more accurate and reliable output phase diagrams.

First Steps:

Our initial steps in generating phase diagrams include preprocessing input data using OpenCV and applying data augmentation techniques to increase the amount of input data. We are experimenting with different neural network models to determine the most suitable one for our project. We are optimistic that our approach, which combines innovative techniques such as data augmentation, neural networks, and OpenCV, will yield accurate and reliable phase diagrams.

Research on Models:

To generate phase diagrams, we have researched various neural network models that can be used to process input data and produce output graphs. We are exploring different models and techniques to obtain the best results. We have experimented with different methods, and though we have not achieved the exact output we want yet, we are getting closer to it. We will continue testing and comparing different models and configurations to fine-tune our approach.

Research on Data Augmentation:

We had a meeting with the expert on the project, or the main stakeholder Peter Lambooij. He helped us plan out how we can re-create the input and output graphs. This is shown in the figures below:

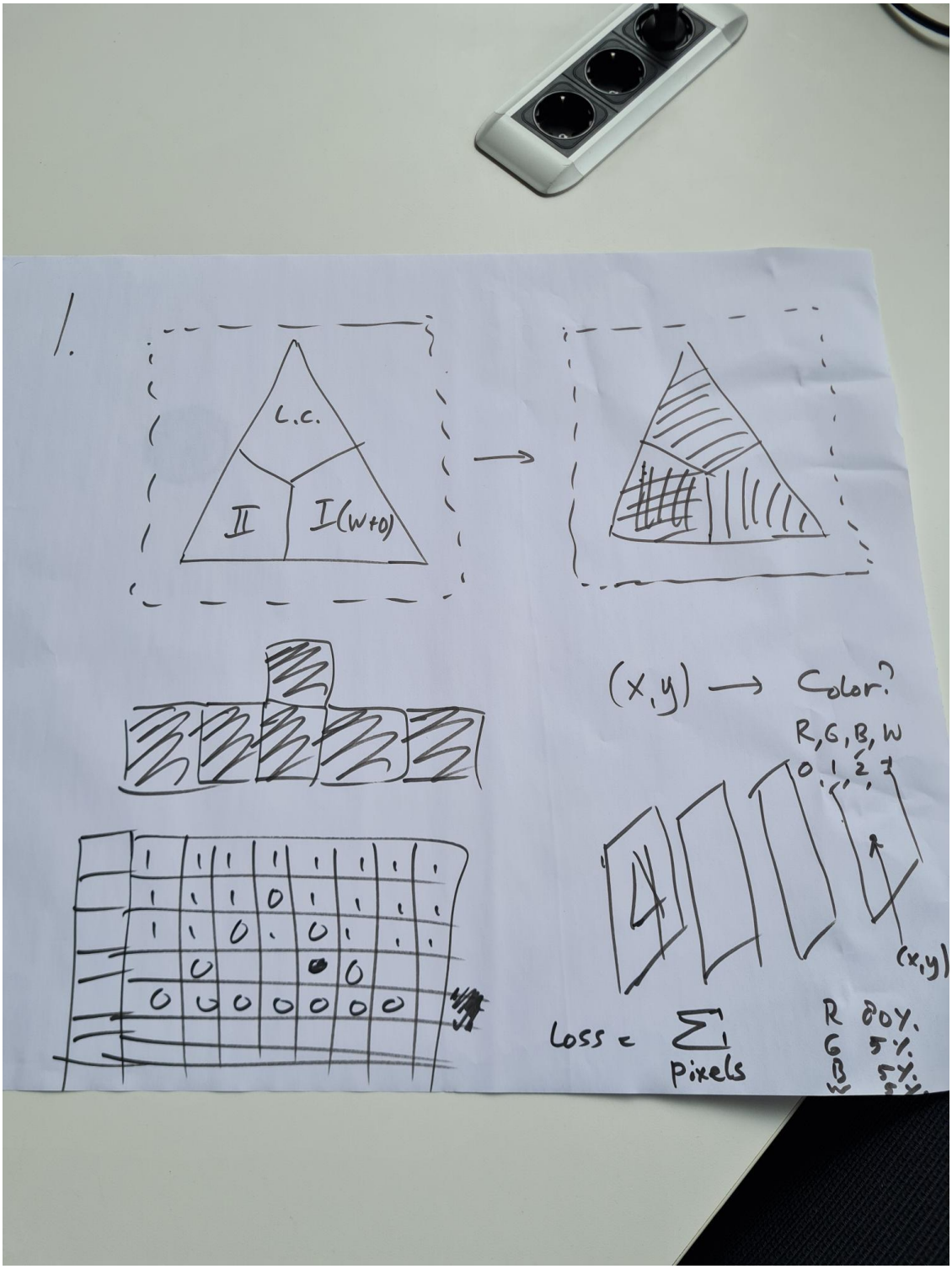

Figure: 1

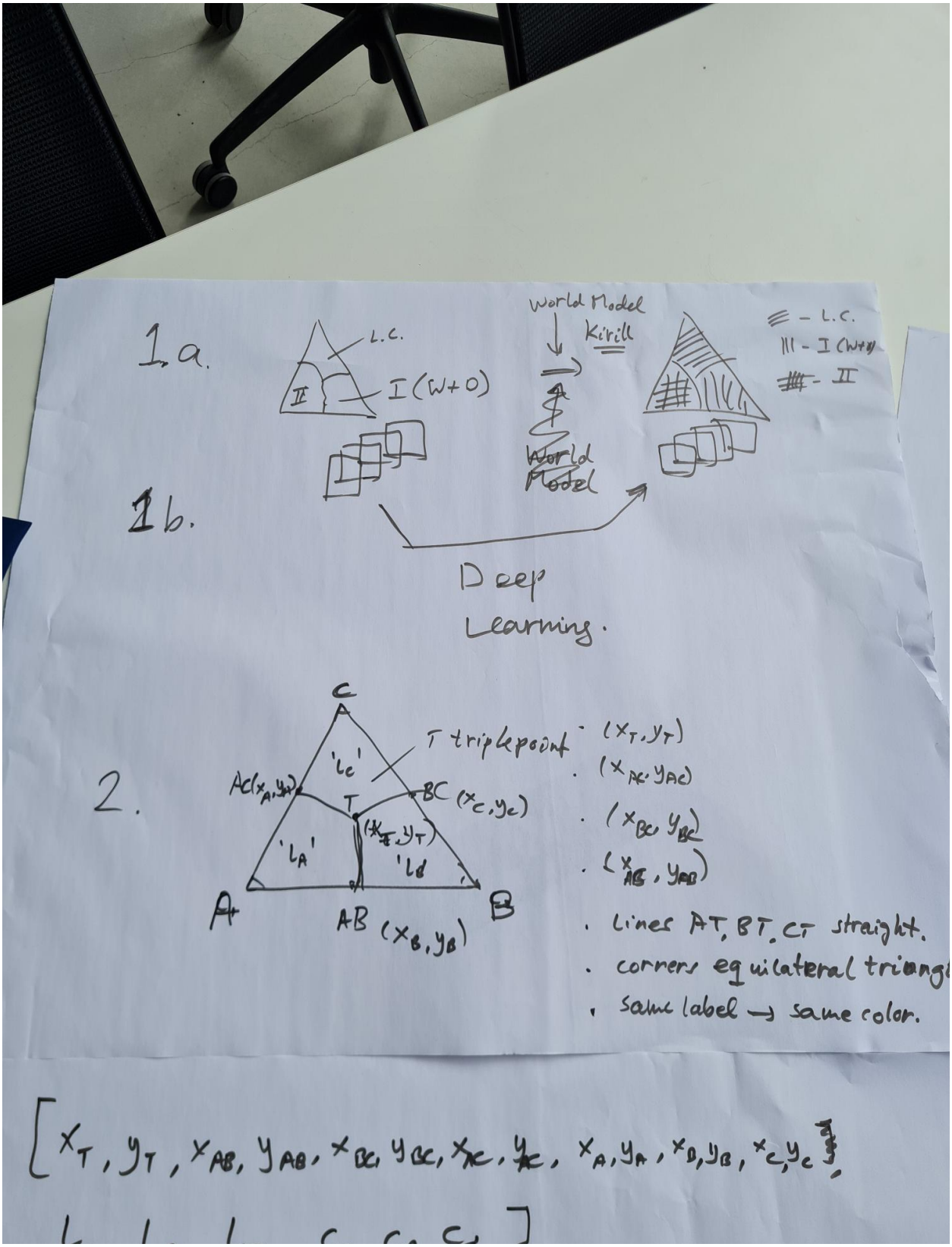
1a.
L.C.
II
I (W+0)
World Model
Kirill
World Model
≡ - L.C.
III - I (W+0)
IIII - II
1b.
Deep Learning.
2.
C
T triplepoint
'Lc'
AC(xA,yA)
BC (xc,yc)
T
(xT,yT)
'LA'
'LB'
A
AB (xB,yB)
B
· (xT,yT)
· (xAC,yAC)
· (xBC,yBC)
· (xAB,yAB)
· Lines AT, BT, CT straight.
· corners equilateral triang
· same label → same color.
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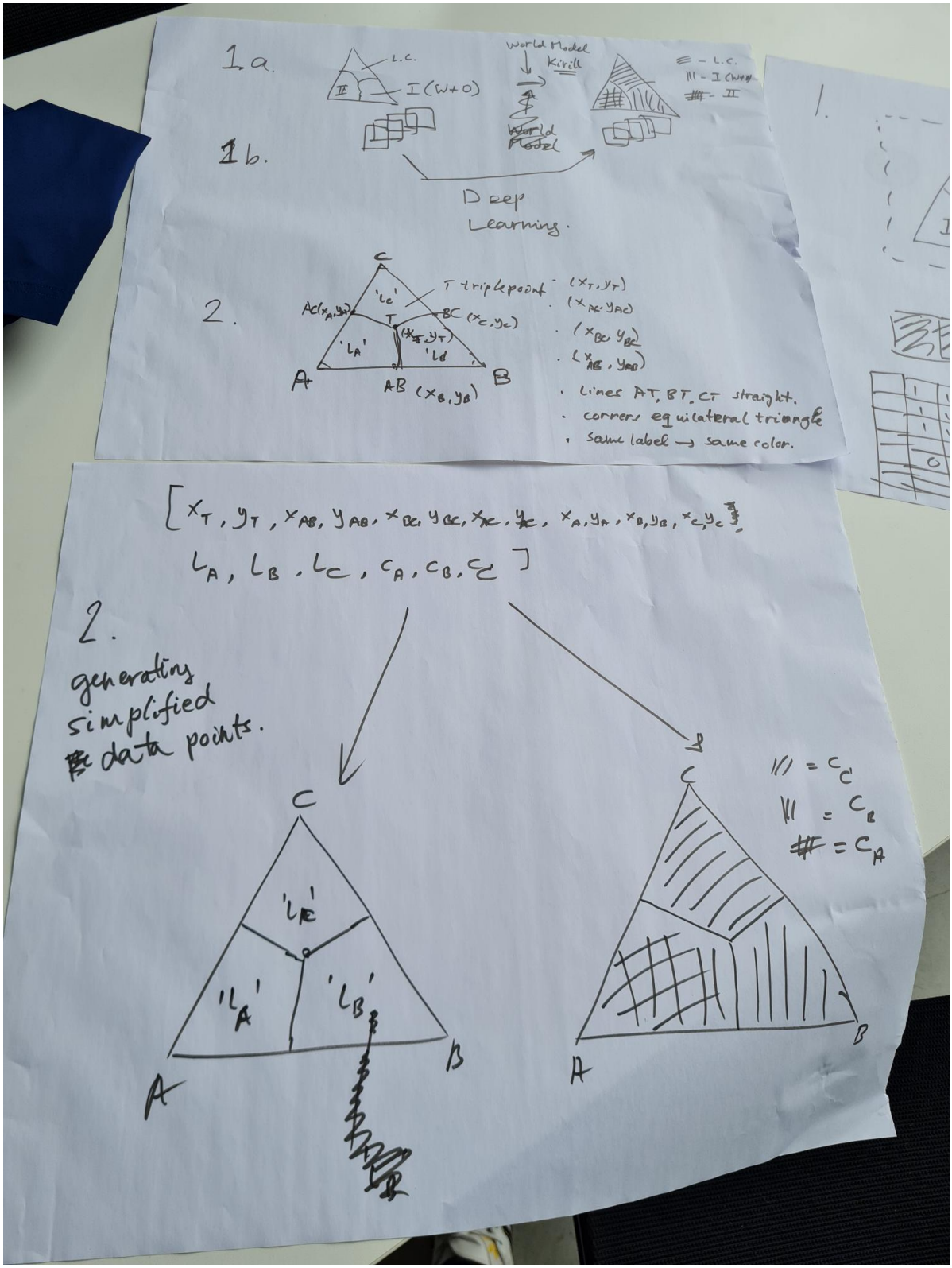
Figure: 2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World Model
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World Model
III - I (W+0)
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AB
B
• Lines AT, BT, CT straight.
• corners equilateral triangle
• same label → same color.
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2.
generating
simplified
data points.
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'LC'
'LA'
'LB'
A
B
III = CC
II = CB
= CA
C
A
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Figure: 3

Conclusion:

Generating phase diagrams for chemical analysis is a challenging task that requires extensive research and experimentation. We have obtained input and output data from our main stakeholder and plan to use data augmentation techniques to create new data from the existing input data. Our initial steps include preprocessing input data with OpenCV and experimenting with different neural network models. Although we have not achieved the exact output we want yet, we are continually fine-tuning our approach to yield accurate and reliable phase diagrams. We believe that our innovative approach, combining data augmentation, neural networks, and OpenCV, will lead us closer to achieving our desired output.