Using Machine Learning to Understand Behavior of F1-ATPase

(1) Andrew Gonzalez, (1) Daniel Martinez
(2) Nathan Suiter, and (3) Dr Sandor Volkan-Kacso
1. Citrus College Student, 2. Peer mentor, 3. Faculty Advisor

Abstract

Adenosine Triphosphate (ATP) is the universal energy currency for all living cells. ATP synthase, comprised of F0-ATPase & F1-ATPase, continually creates ATP by using the momentum from the flow of protons to its F0-ATPase rotor. F1-ATPase which is connected to F0-ATPase by a base, creates ATP from both ADP and a Phosphorus atom. We aim to create an AI model that will allow us to examine and predict the rotation cycle of ATP synthase.

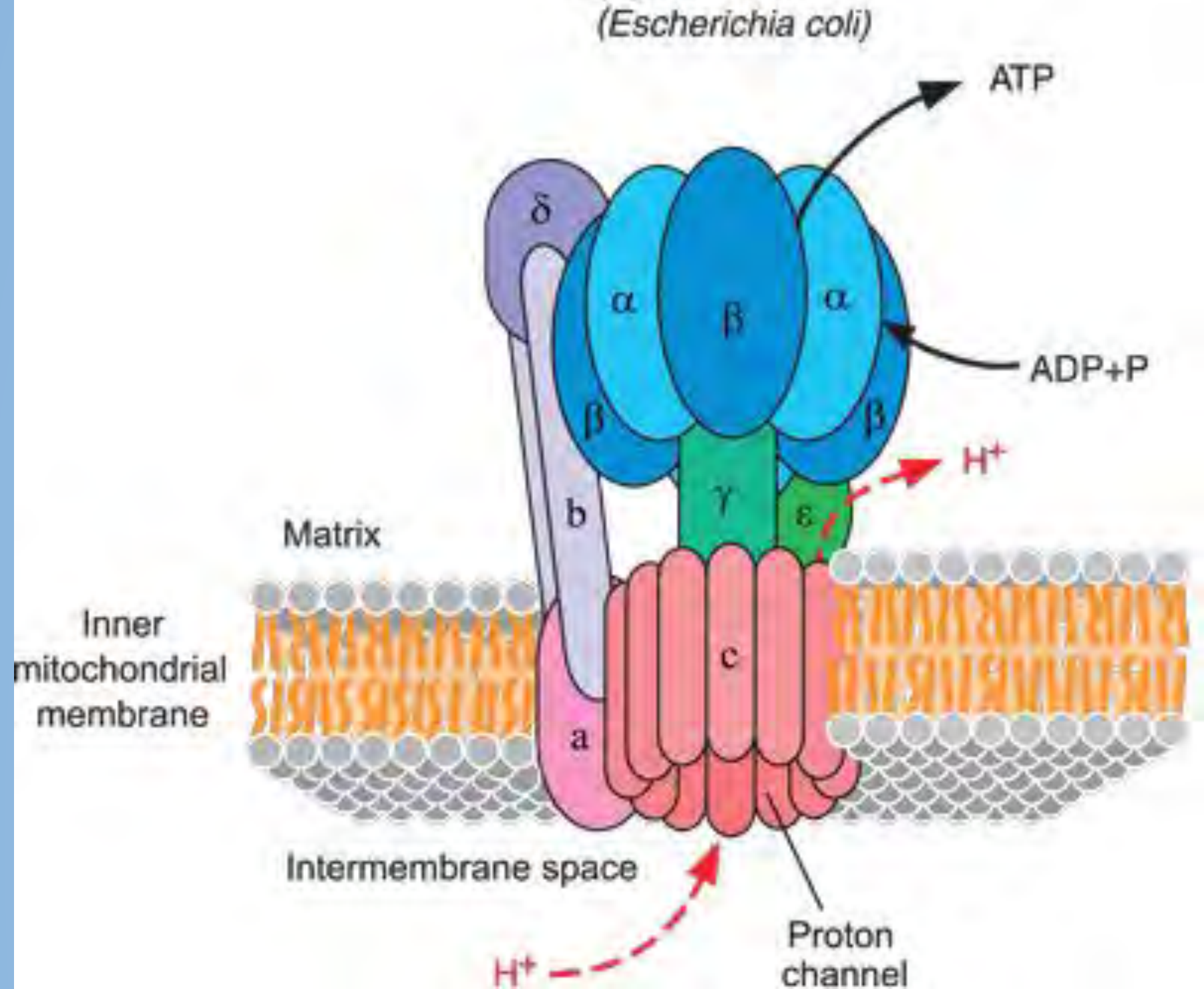

Figure 1 (above). 2D model rendering of F1-ATPase (taken from https://creation.com/atp-synthase)

Introduction

This study employs machine learning to understand the behavior of F1-ATPase, using real data to find patterns and hidden characteristics. The rotation of ATP synthase occurs in 120 degree steps which we refer to as transition states, and resting states which we refer as dwell states. Using previous data, we aimed to build a machine learning model that will identify and possibly predict the current state of ATP synthase at any given time. Analyzing the transition states and dwell states separately can allow researchers to examine the chemical compounds and kinetics of ATP synthase.

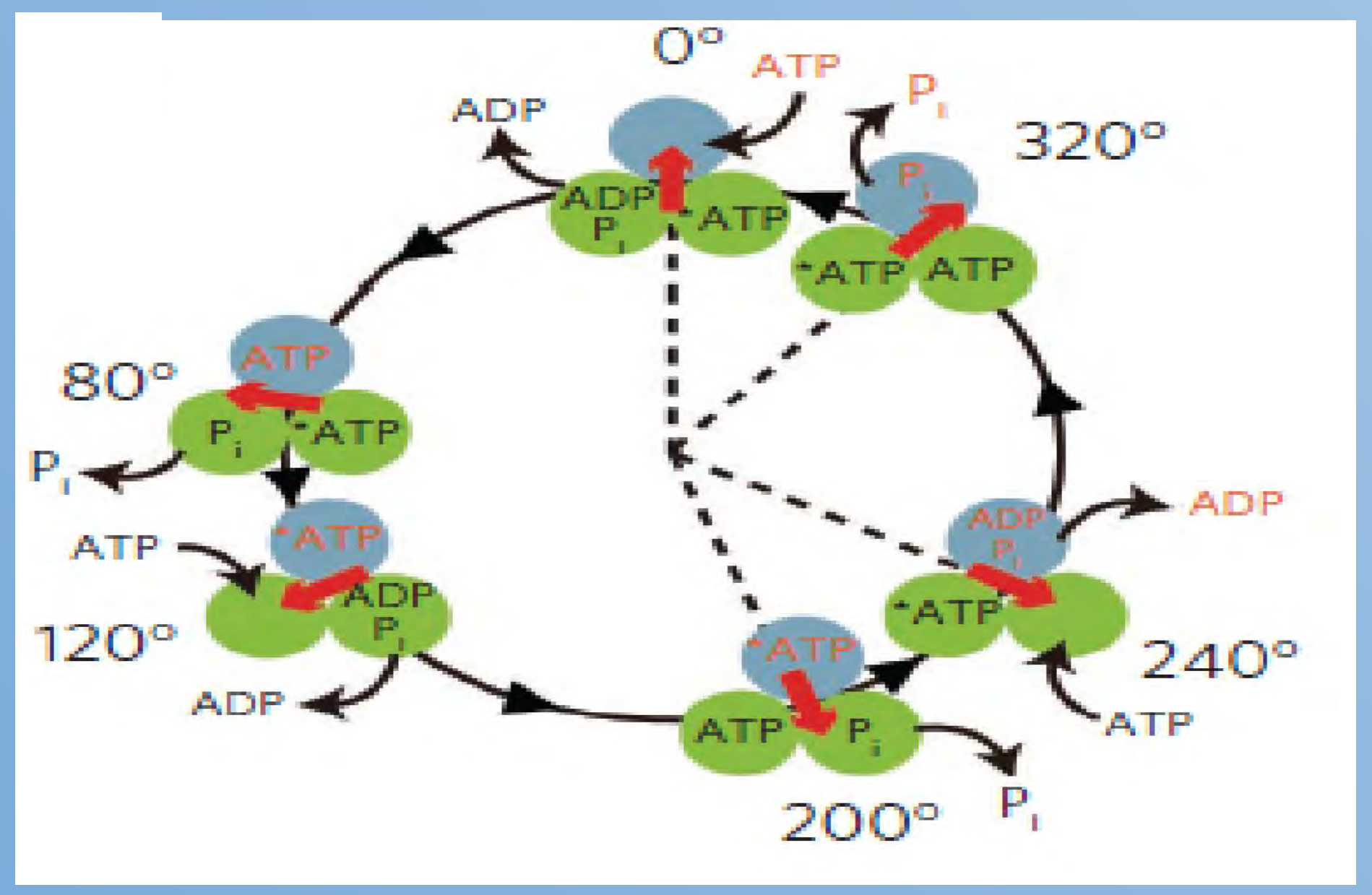

Figure 2, Rotation of FATPase

Methods

Classification:

- Using data points taken by hand, we will train our model to identify where the transition points start and where they end.

Regression:

- Assists in predicting the transitions and dwells of ATP synthase as time increases.

MATLAB:

- Used for plotting our data into something we can understand.

Scikit-learn:

- Used for its various tools and its classification and regression models

Pandas Library:

- Used to read our files and store them into data we can manipulate.

NumPy:

- Used to make calculations on our data in an efficient manner.

Results

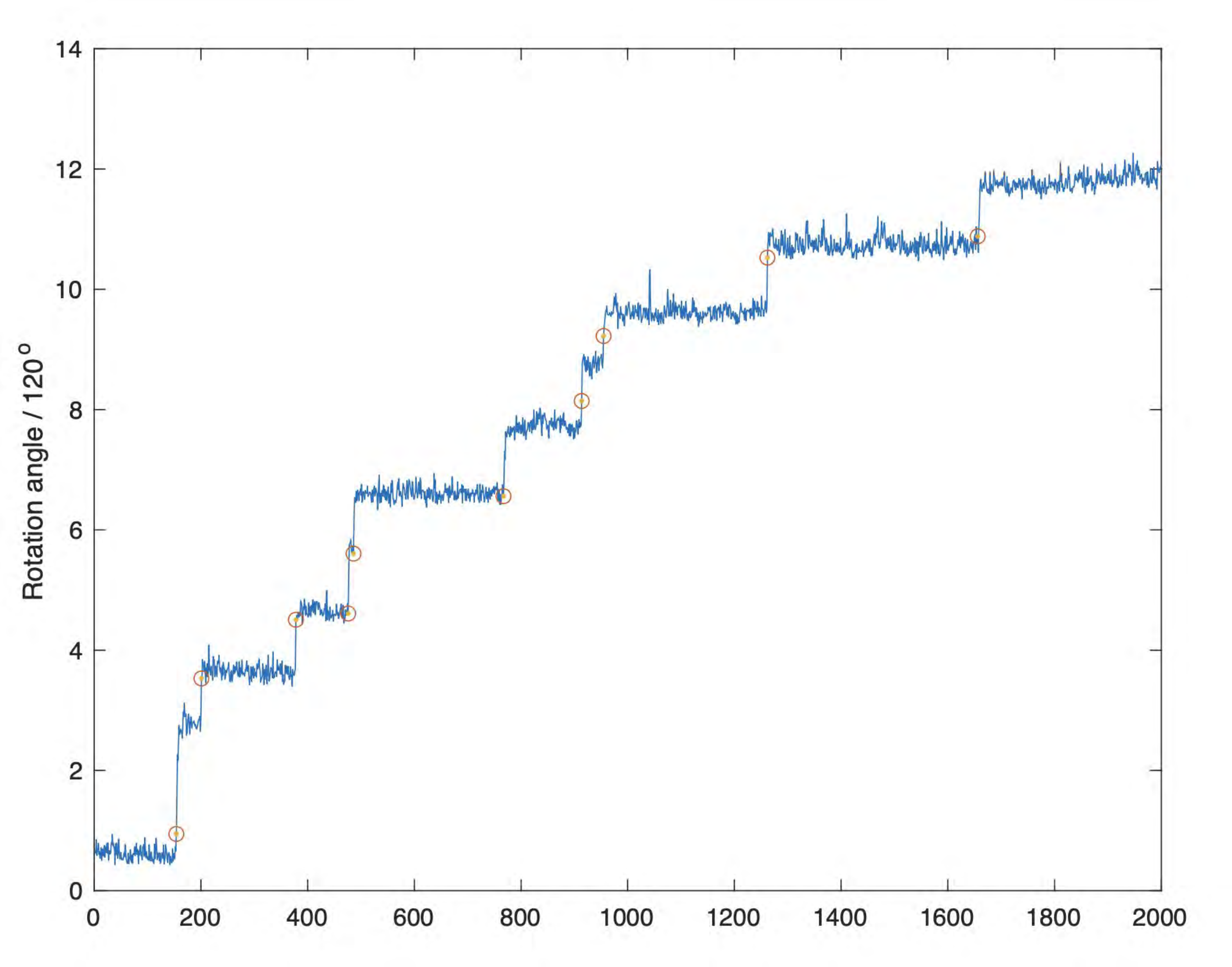

Figure 3 (transition points in red).

Results Continued

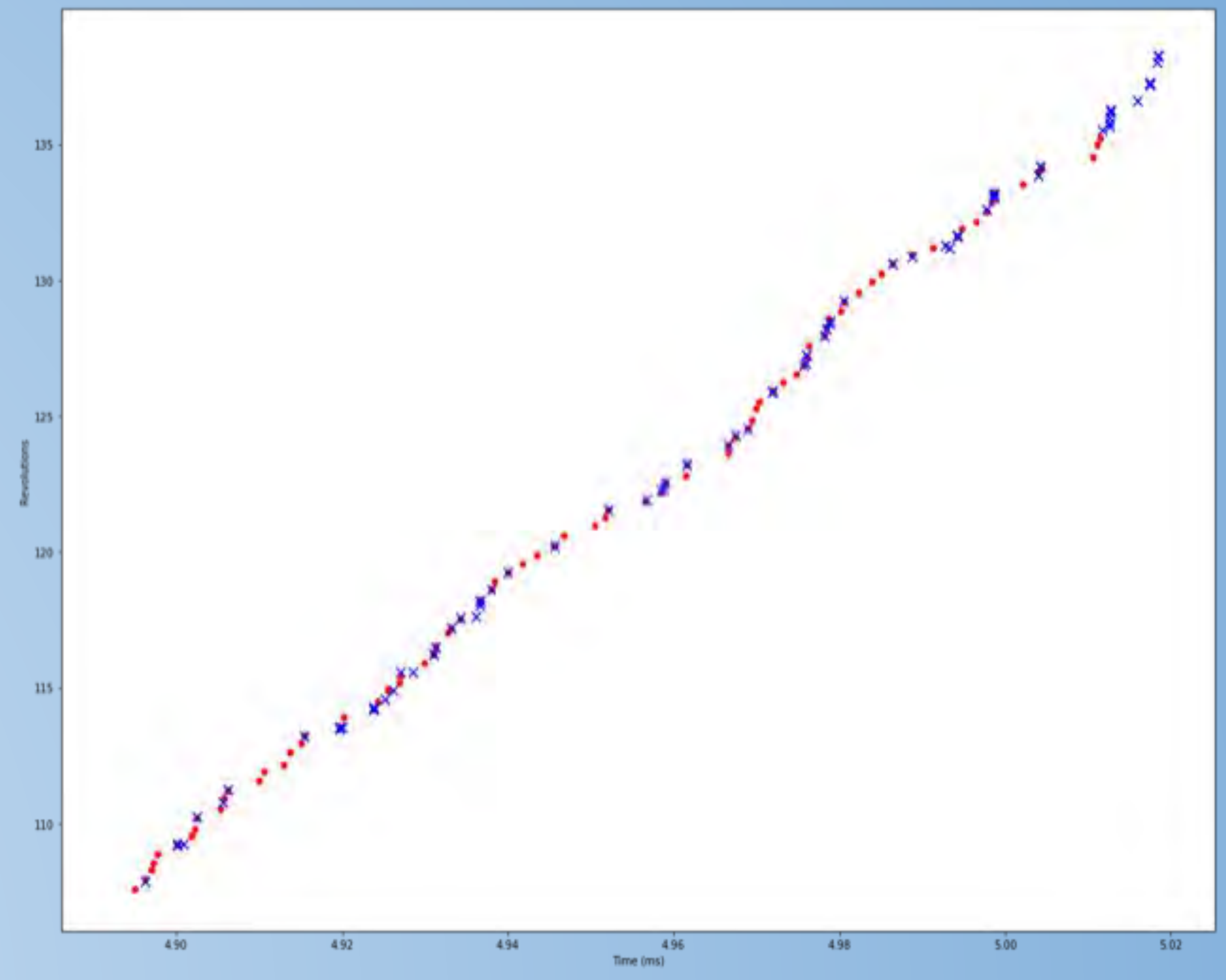

Figure 4 (red is real data blue is predicted)

Using a gradient boosting classifier model, we were able to come up with an AI that marked some of the transition points, however some were still off mark.

Conclusions

- While the AI model we created produced some transition points, the model was inconsistent with locating the starting and ending points.
- The stochastic nature of cellular energy production and the limitations of the dataset may have contributed to these inconclusive results.
- To advance the understanding of F1-ATPase and its implications, future research endeavors are recommended that involve larger and more comprehensive datasets and the exploration of advanced machine learning algorithms.

Acknowledgements

The presenters would like to thank Dr. Sandor Volkan-Kacso from Azusa Pacific University, Nathan Suiter, Hiroshi Ueno & Hiroyuki Noji from the University of Tokyo, the Citrus College Foundation, and Victoria Dominguez and Monica Hernandez of the Citrus College Summer Research Experience program for this research opportunity.

Alternate Text

Andrew Gonzalez and Daniel Martinez

Azusa Pacific University

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