[COGS 9] Discussion Reading 1, Python Basics

Reading Quiz 1 on 12th July (Wed)

Donoho's six divisions

- Data Gathering, Preparation, and Exploration
- Data Representation and Transformation
- Computing with Data
- Data Modeling
- Data Visualization and Presentation
- Science about Data Science

Data Gathering, Preparation, and Exploration

For example, a data team can gather data

about patient demographics, medical history and drug efficacy, from clinical trials, electronic health record, and public datasets,

Prepare the data,

by data cleaning, such as removing any missing or inconsistent values,

And explore the data,

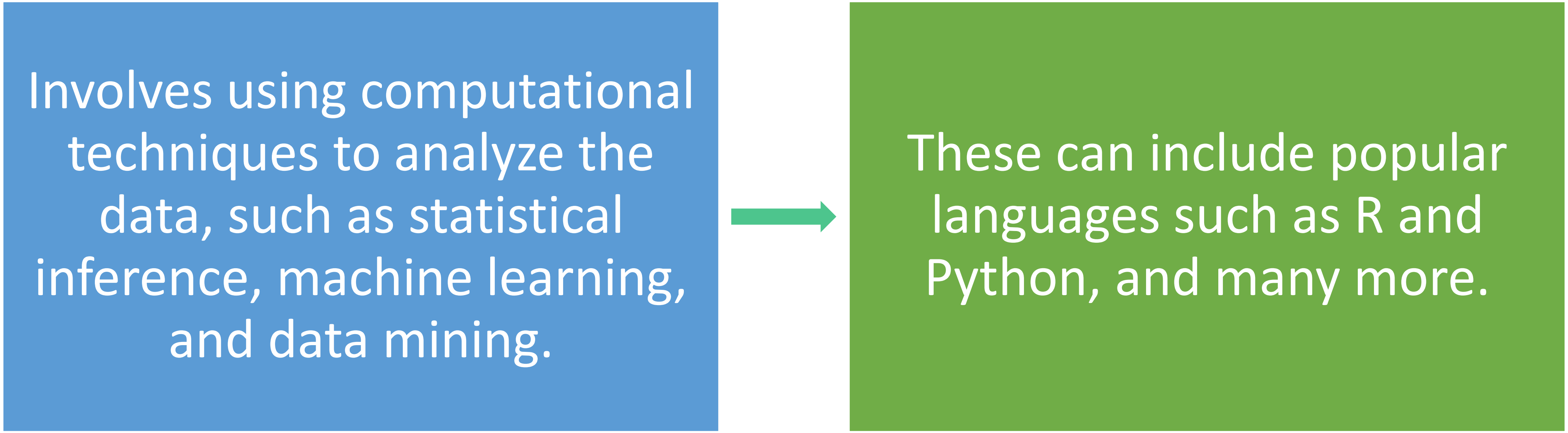
by creating visualizations, such as histograms and scatter plots,
to understand the distribution and identify patterns from the data.

Data Representation and Transformation

After exploring the data, the team would represent and transform the data in a way that is suitable for analysis and modeling.

This could include feature engineering, normalization, and dimensionality reduction.

Computing with Data



Involves using computational techniques to analyze the data, such as statistical inference, machine learning, and data mining.

These can include popular languages such as R and Python, and many more.

Data Visualization and Presentation

The data team would create visual representations of the data, such as heatmaps and bar charts, to make it easier to understand and interpret the data.

For example, they could create interactive dashboards that allow the medical team to explore the data and gain insights, and also prepare the results of the project in a way that is easy to understand and present to stakeholders.

Science about Data Science

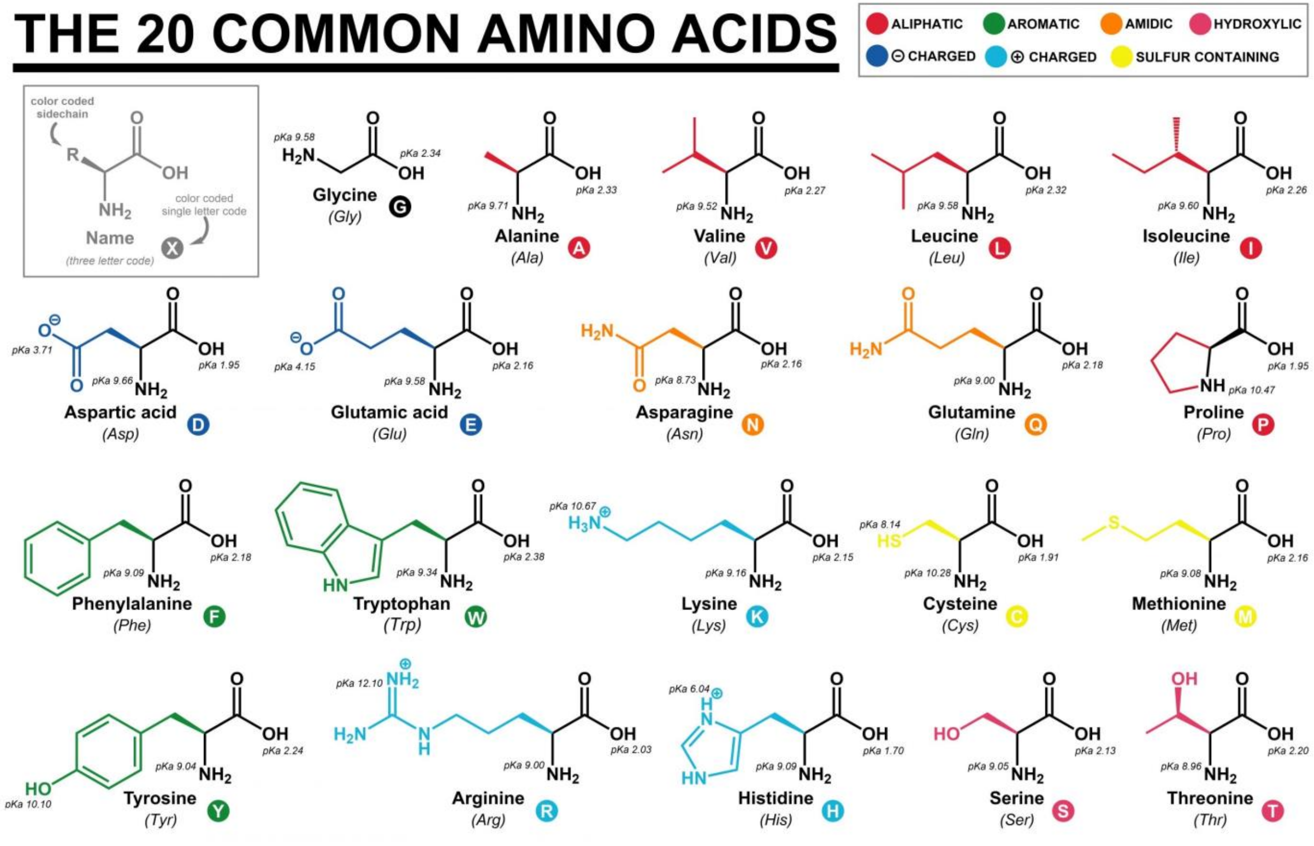
Tukey proposed that ‘a science of data analysis’ exists and should be recognized as among the most complicated of all sciences.”

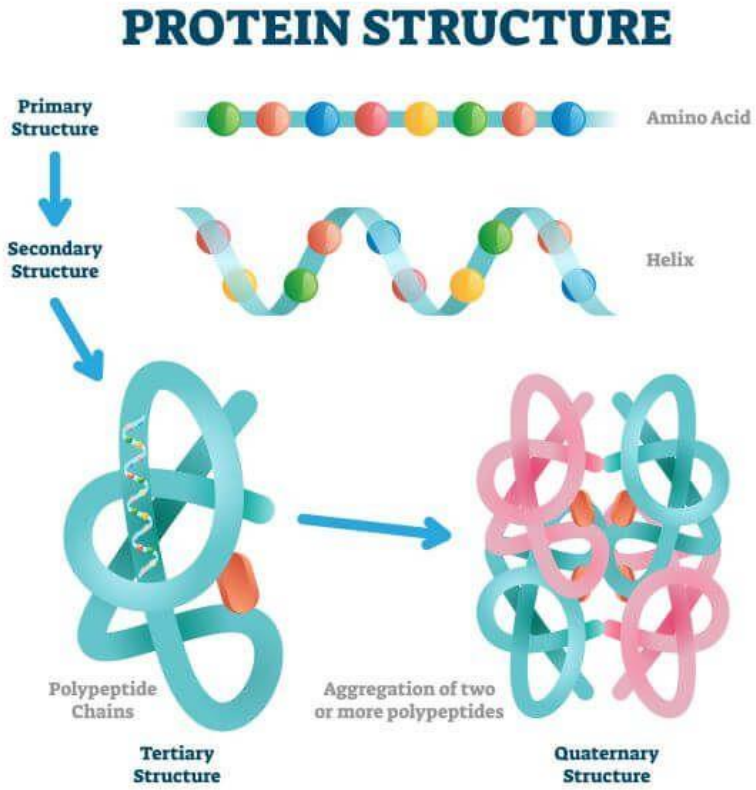
It involves monitoring the performance of the model, validating the findings, and understanding the ethical and legal implications of the results.

Additionally, it involves staying current with the latest developments and trends in data science and being able to reflect on the processes and methods used throughout the project.

Background information

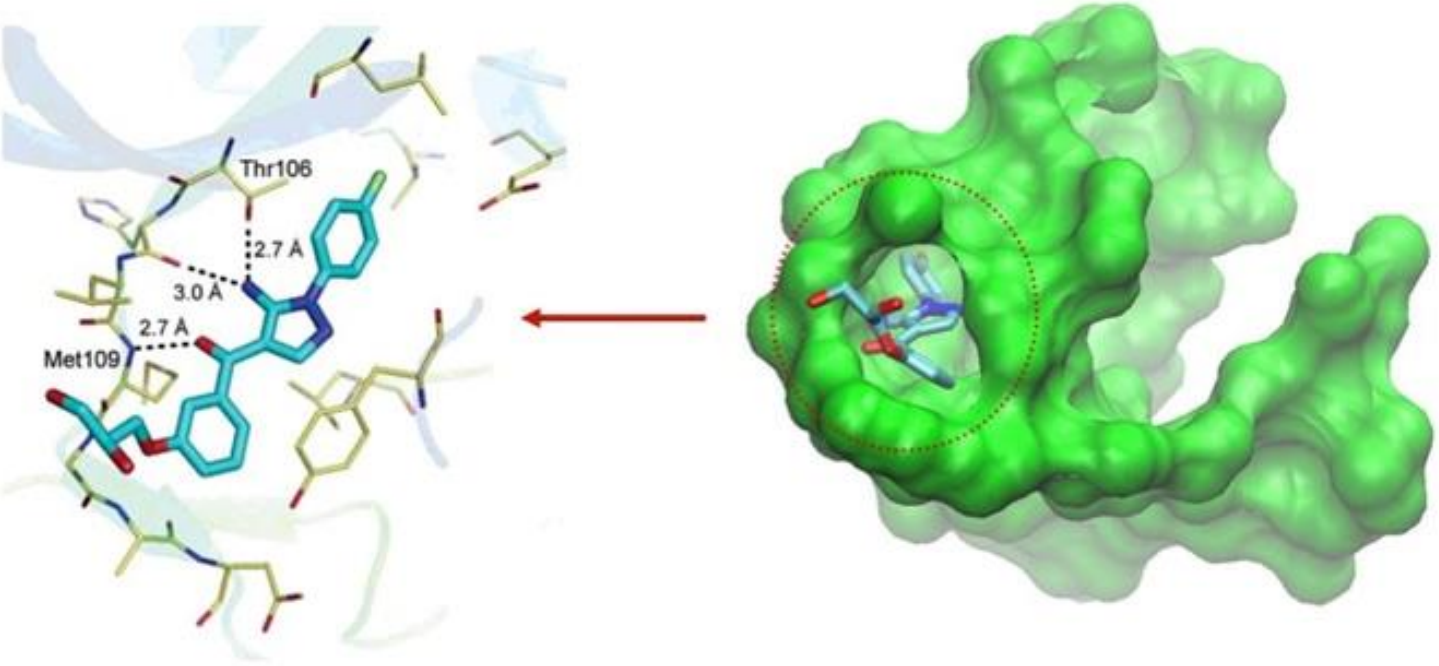
- Let’s go through a data science project from my life (Spent 2 years :))
- You do not need to know anything about the nitty-gritties. This is just an example to show you a data science project from the perspective of Donoho’s six divisions
- Problem: Predicting the amino acids of a protein (from sequence information alone) that bind to most drugs
- GitHub: https://github.com/devalab/BiRDS

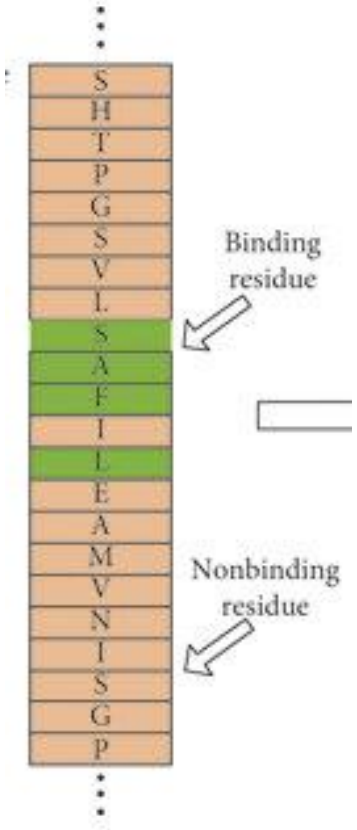




Background Information

Data Gathering, Preparation and Exploration

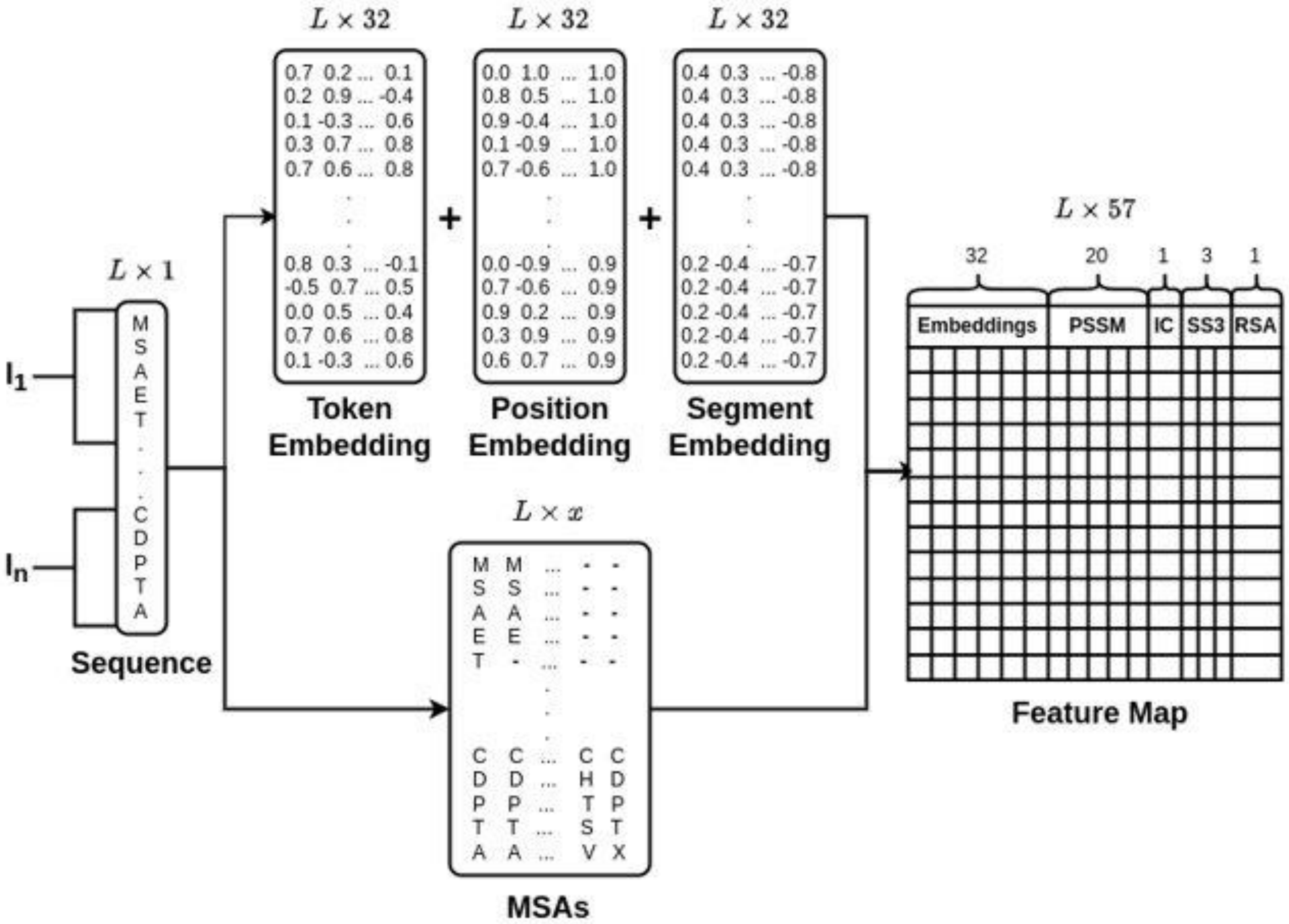




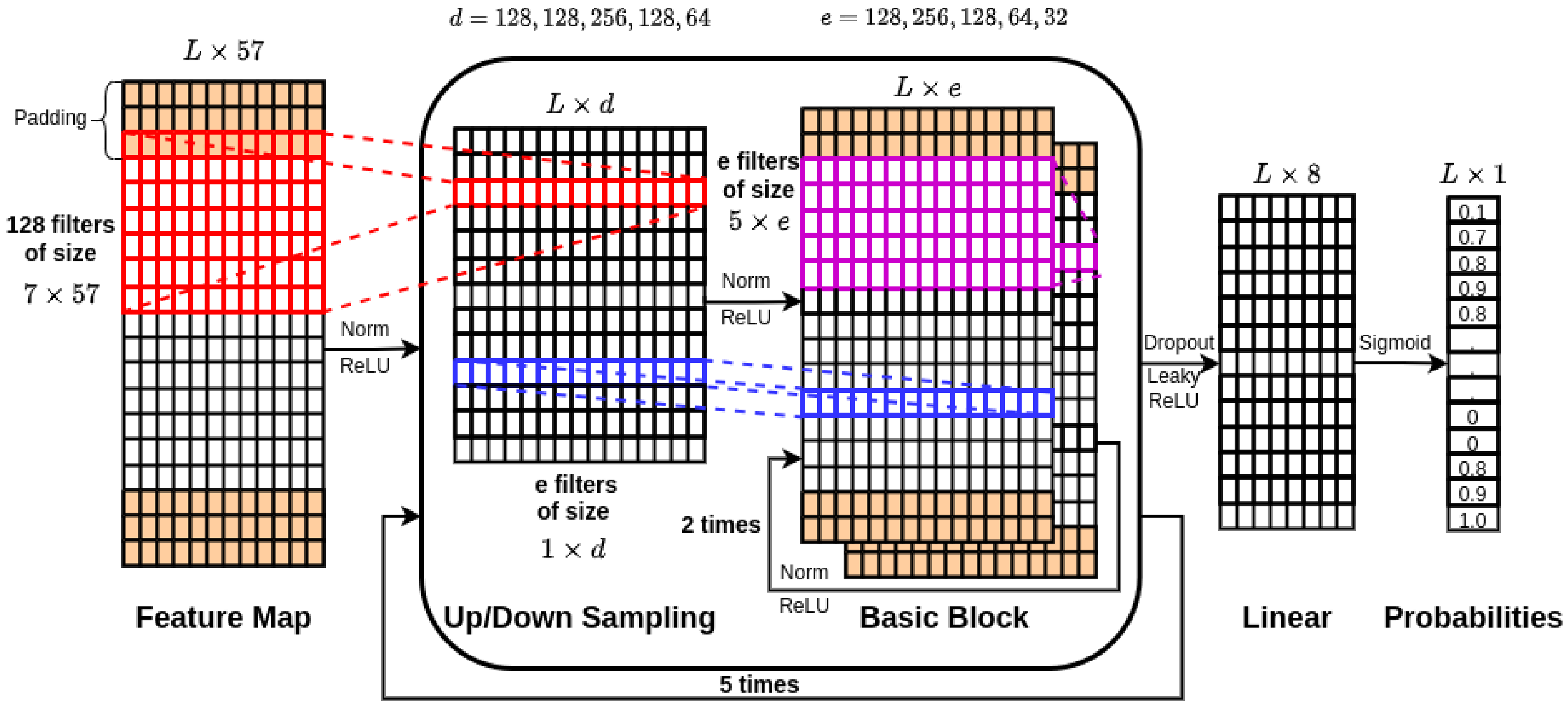
Data Representation and Transformation

- Extracting information from sequences
  - Using some NLP techniques
  - Using sequences similar to current sequence to gather information
  - Using some property predictions from other ML models
- Storage
  - Numpy arrays
  - Zstd compression

Computing with Data



Data Modeling



Data Visualization and Presentation

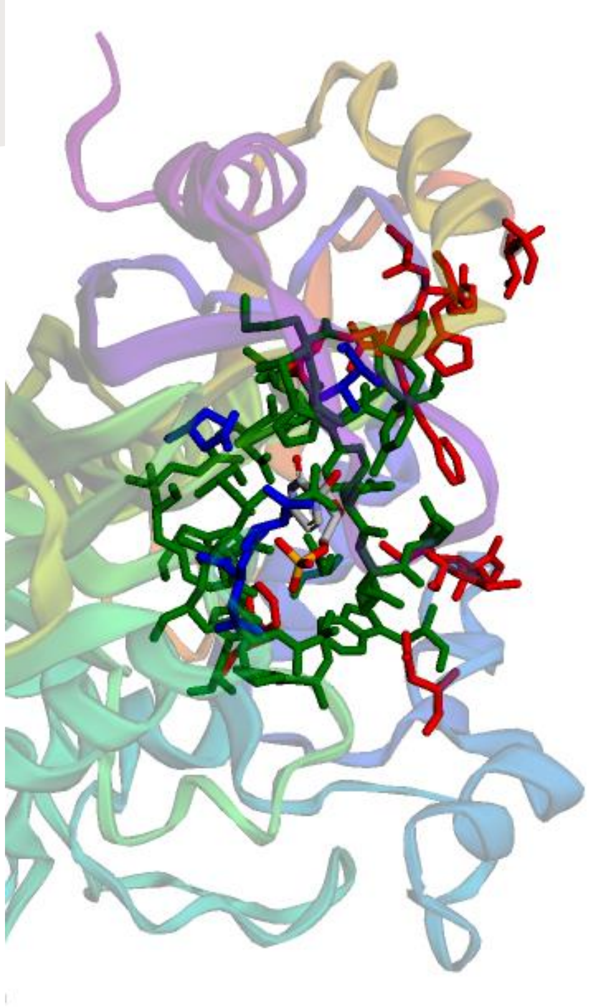
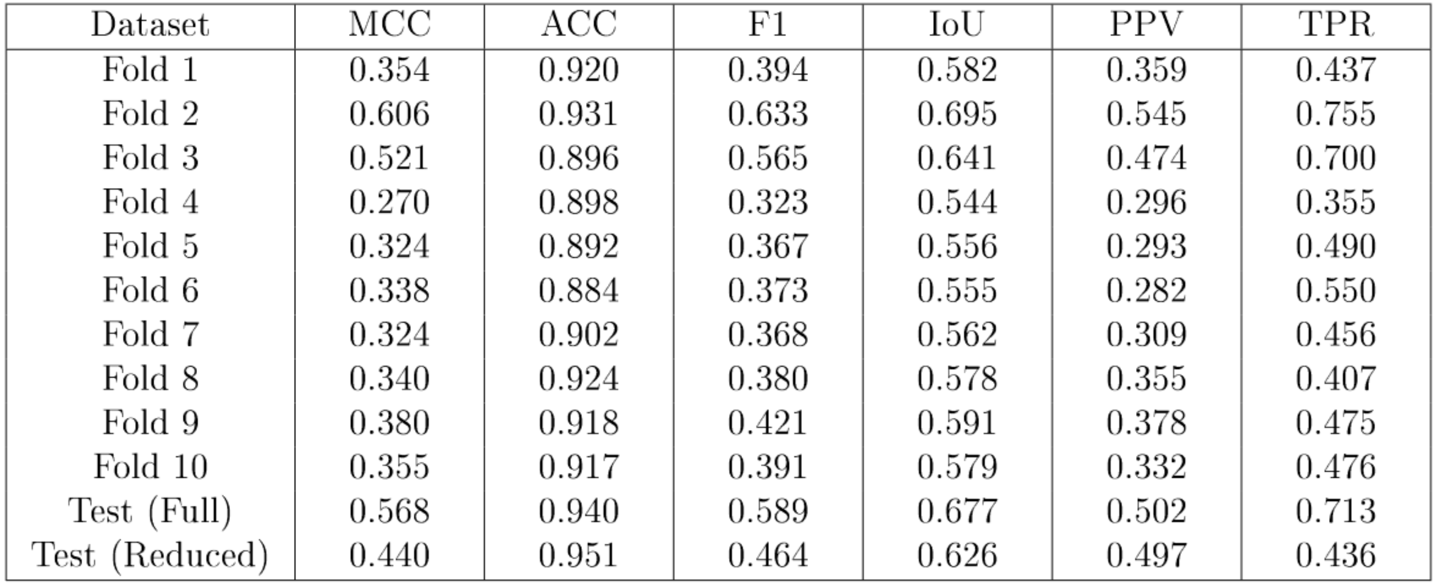


Table 1: Validation and test results



Dataset	MCC	ACC	F1	IoU	PPV	TPR
Fold 1	0.354	0.920	0.394	0.582	0.359	0.437
Fold 2	0.606	0.931	0.633	0.695	0.545	0.755
Fold 3	0.521	0.896	0.565	0.641	0.474	0.700
Fold 4	0.270	0.898	0.323	0.544	0.296	0.355
Fold 5	0.324	0.892	0.367	0.556	0.293	0.490
Fold 6	0.338	0.884	0.373	0.555	0.282	0.550
Fold 7	0.324	0.902	0.368	0.562	0.309	0.456
Fold 8	0.340	0.924	0.380	0.578	0.355	0.407
Fold 9	0.380	0.918	0.421	0.591	0.378	0.475
Fold 10	0.355	0.917	0.391	0.579	0.332	0.476
Test (Full)	0.568	0.940	0.589	0.677	0.502	0.713
Test (Reduced)	0.440	0.951	0.464	0.626	0.497	0.436

Science about Data Science

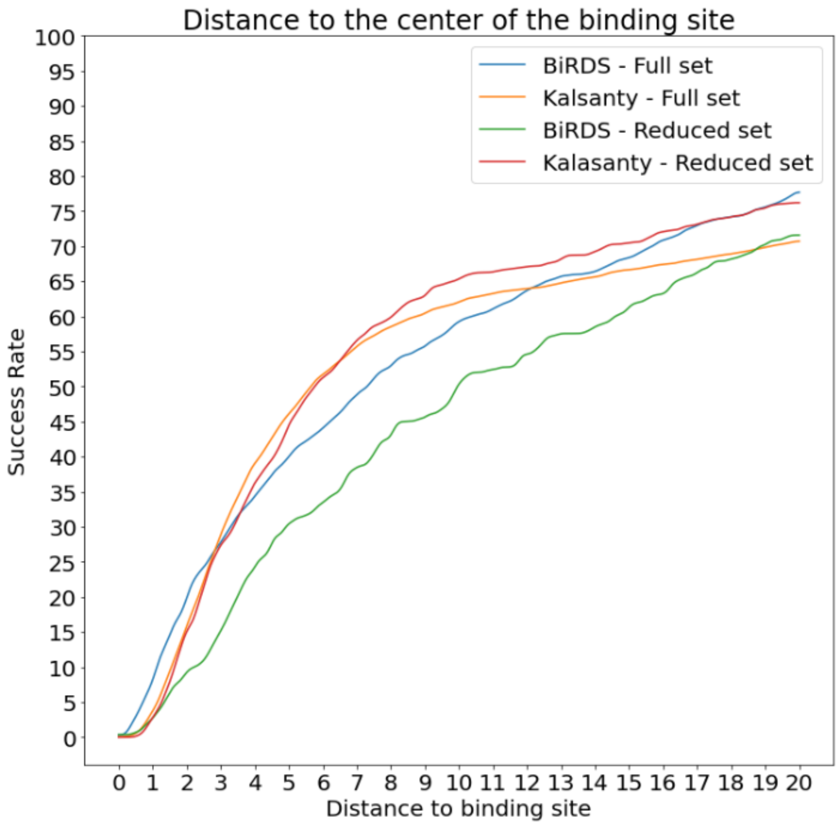


Figure 6: Success rate plot for various DCC thresholds on the test set after averaging the predictions of the 10 models