UNIVERSITY of WASHINGTON

rateExtrapolation.py

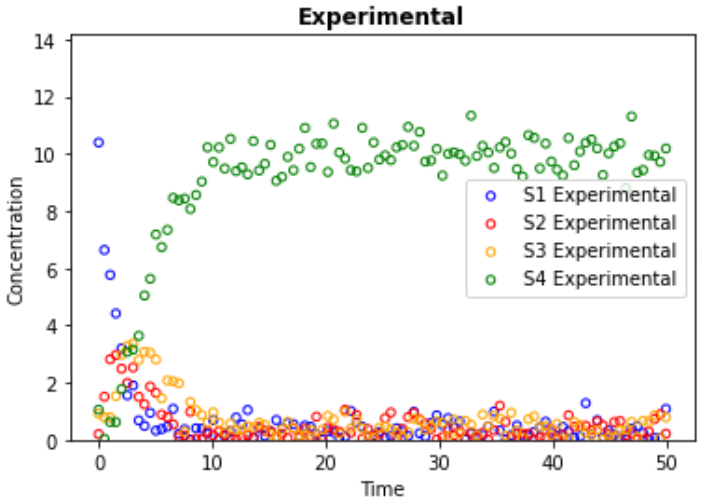
simple reaction rate extrapolation from experimental data

BIOEN537
Sarah Wait
Fall 2021

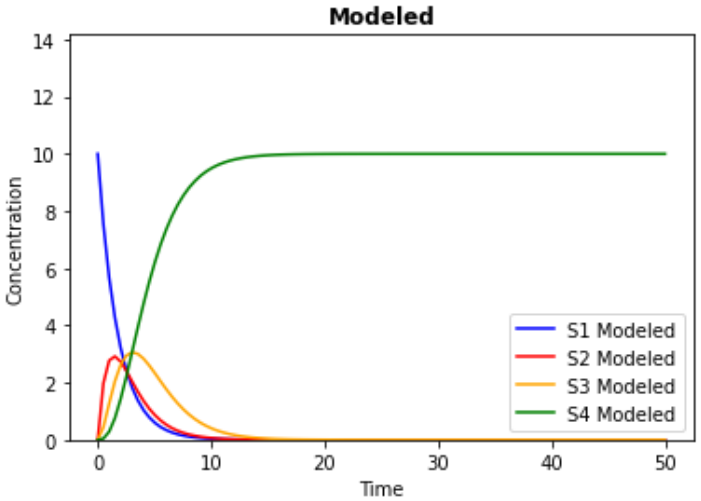
Background: *Empirical data generation and model fitting steps are currently segmented.*

Experimentalists

Computationalists

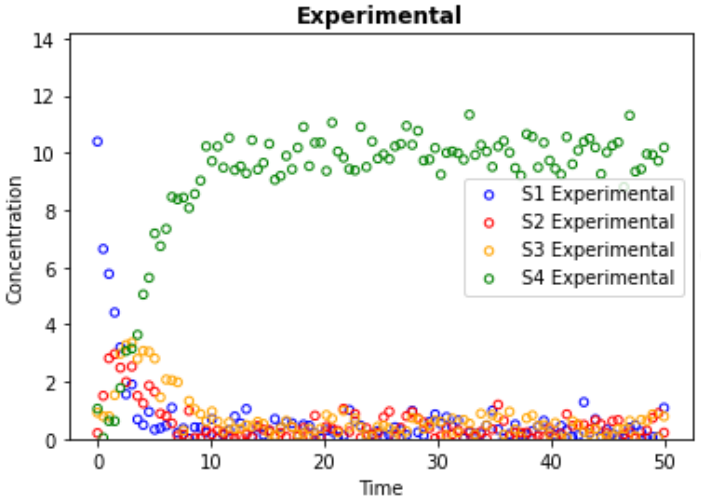


- Parameter Fitting
- Cross Validation
- Summary of Model Fitting



Goal: *Create a simplified function that an experimentalist can utilize to quickly model simple reactions*

Experimentalists



rateExtrapolation.py

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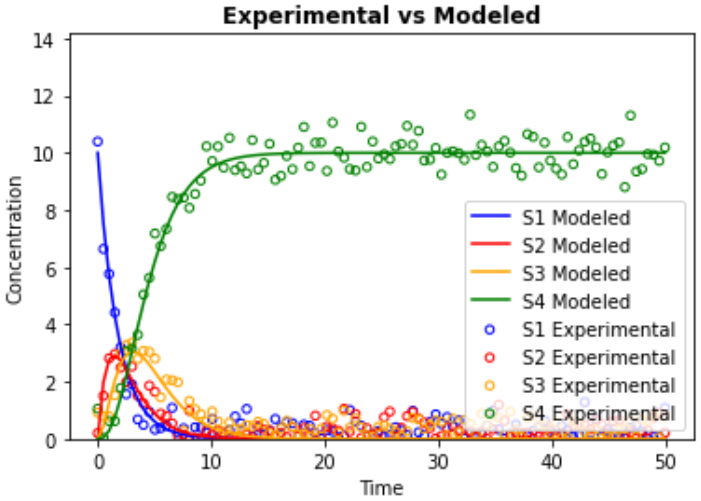
- Cross Validation
- Summary of Model Fitting



Intended Users: *The intended users are experimentalists who have some experience in coding.*

Experimentalists (& computationalists)

Experience coding in Python

Ideally, understands data structures such as float, int, string etc.

Able to import and execute packages in python

e.g. import pandas as pd
& y = rateExtrapolation(data)

Able to write Tellurium Antimony String

e.g. antimony = """
*S1 -> S2; k1*S1;*
*S2 -> S3; k2*S2;*
S1 =10; S2 = 0; S3 = 0;
k1= 0; k2 =0 """

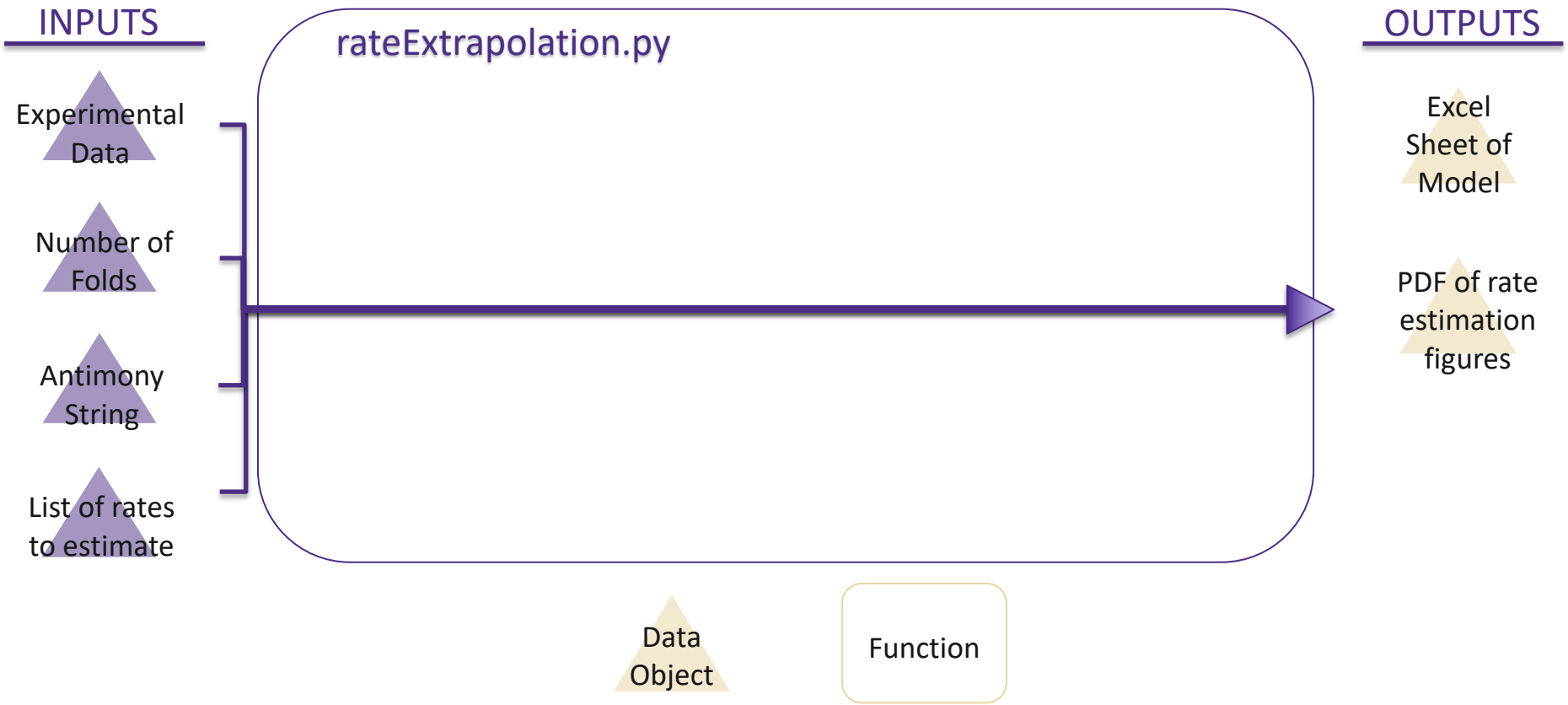
Use cases: *Experimentalist does all steps including data generation, code execution, and analysis of results.*

- User generates time course data for biolgical network of interest

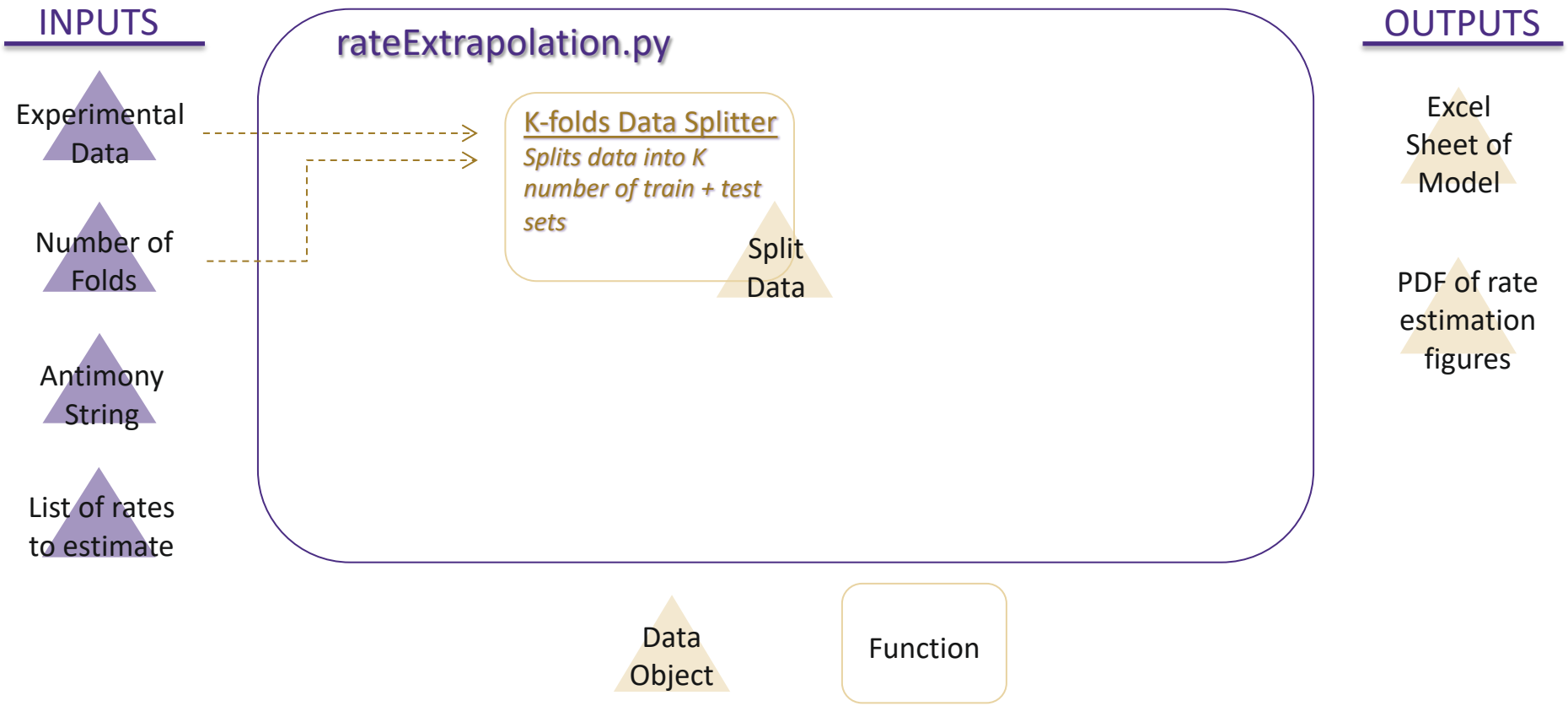
- User opens python notebook
- loads the rateExtrapolation function
- User provides input and executes function

- User reads provided results from the function
- Accepts or rejects the extrapolated rates

Design


INPUTS
Experimental Data
Number of Folds
Antimony String
List of rates to estimate
rateExtrapolation.py
OUTPUTS
Excel Sheet of Model
PDF of rate estimation figures
Data Object
Function

Design


INPUTS
Experimental Data
Number of Folds
Antimony String
List of rates to estimate
rateExtrapolation.py
K-folds Data Splitter
Splits data into K number of train + test sets
Split Data
OUTPUTS
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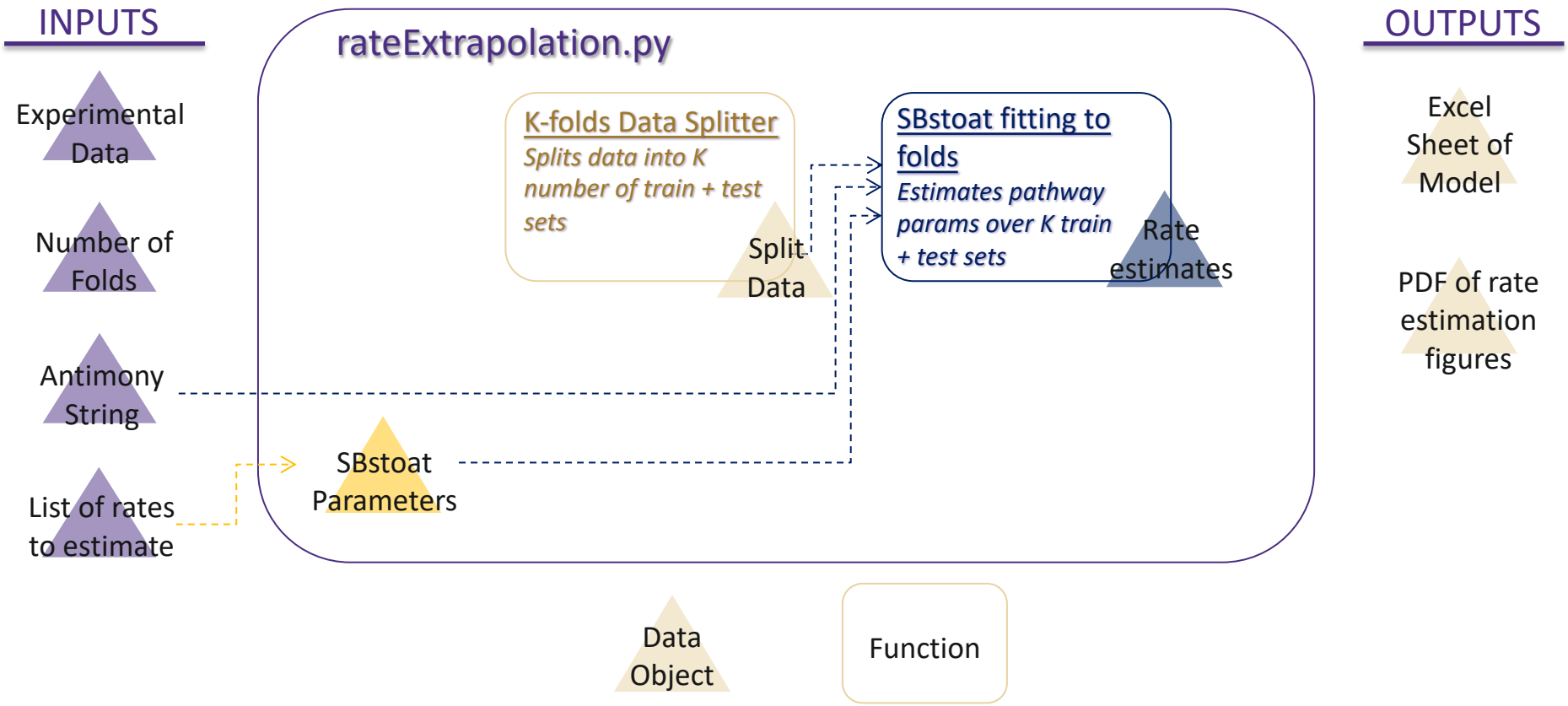
Data Object
Function

Design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Split Data
SBstoat fitting to folds
Estimates pathway params over K train + test sets
Rate estimates
SBstoat Parameters
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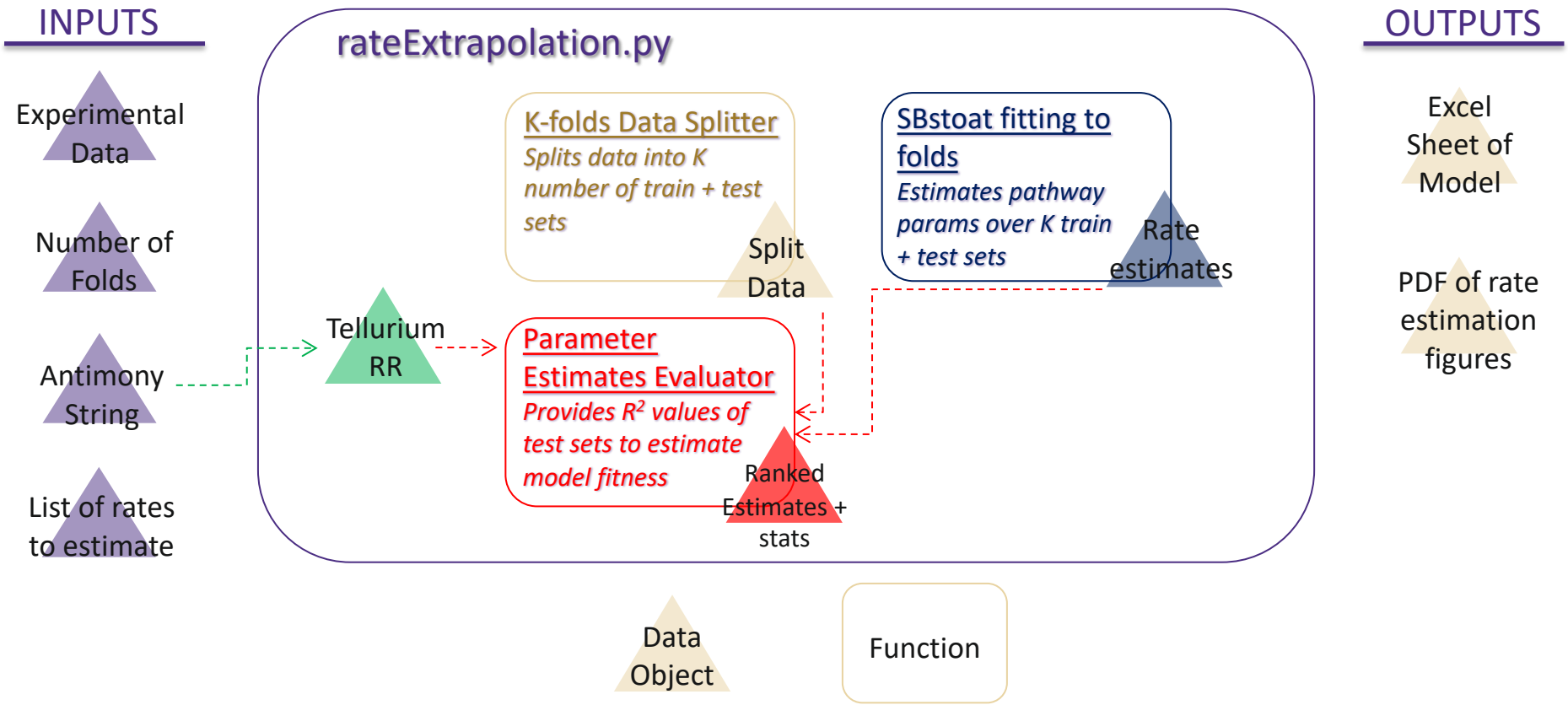
Design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Tellurium RR
Parameter Estimates Evaluator
Provides R^2 values of test sets to estimate model fitness
Ranked Estimates + stats
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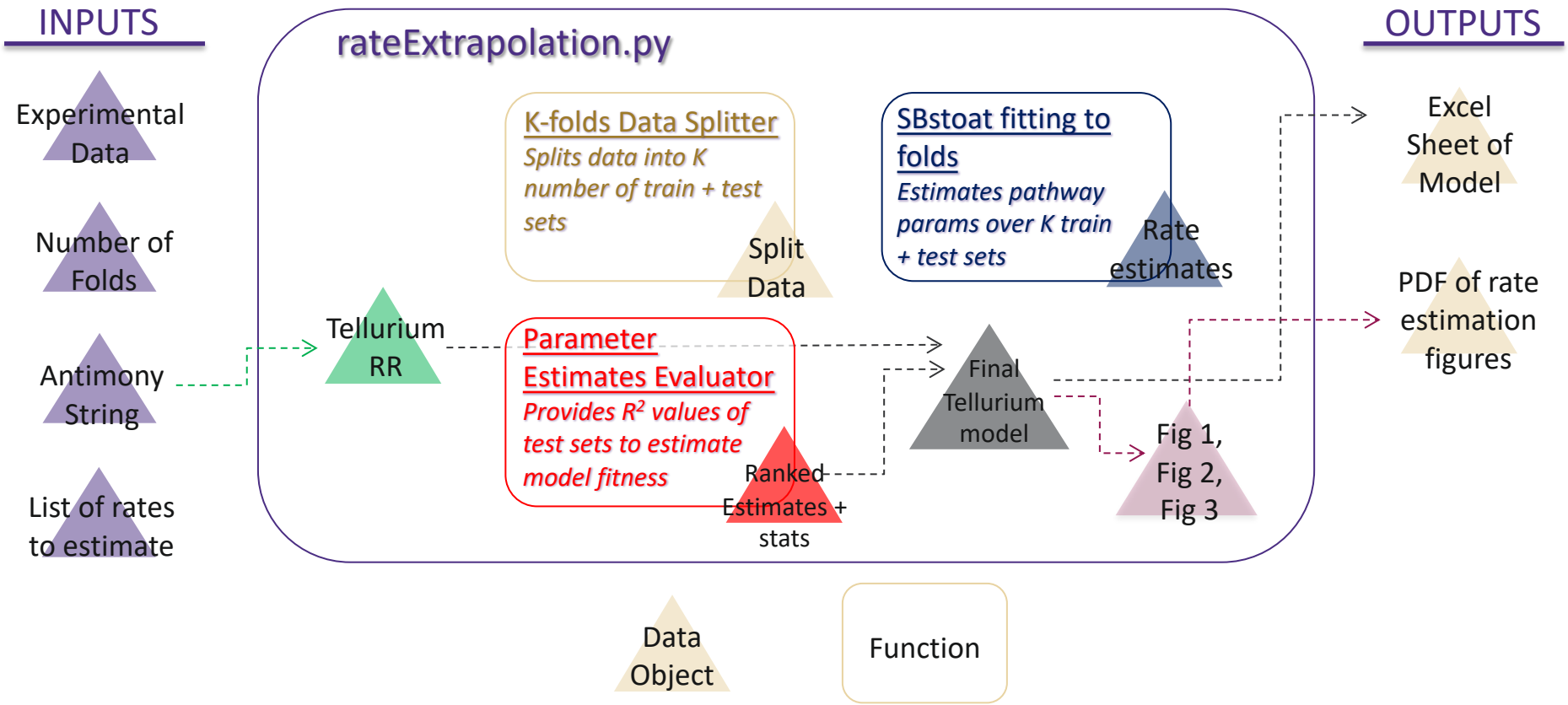
Design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Final Tellurium model
Fig 1, Fig 2, Fig 3
OUTPUTS
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Data Object
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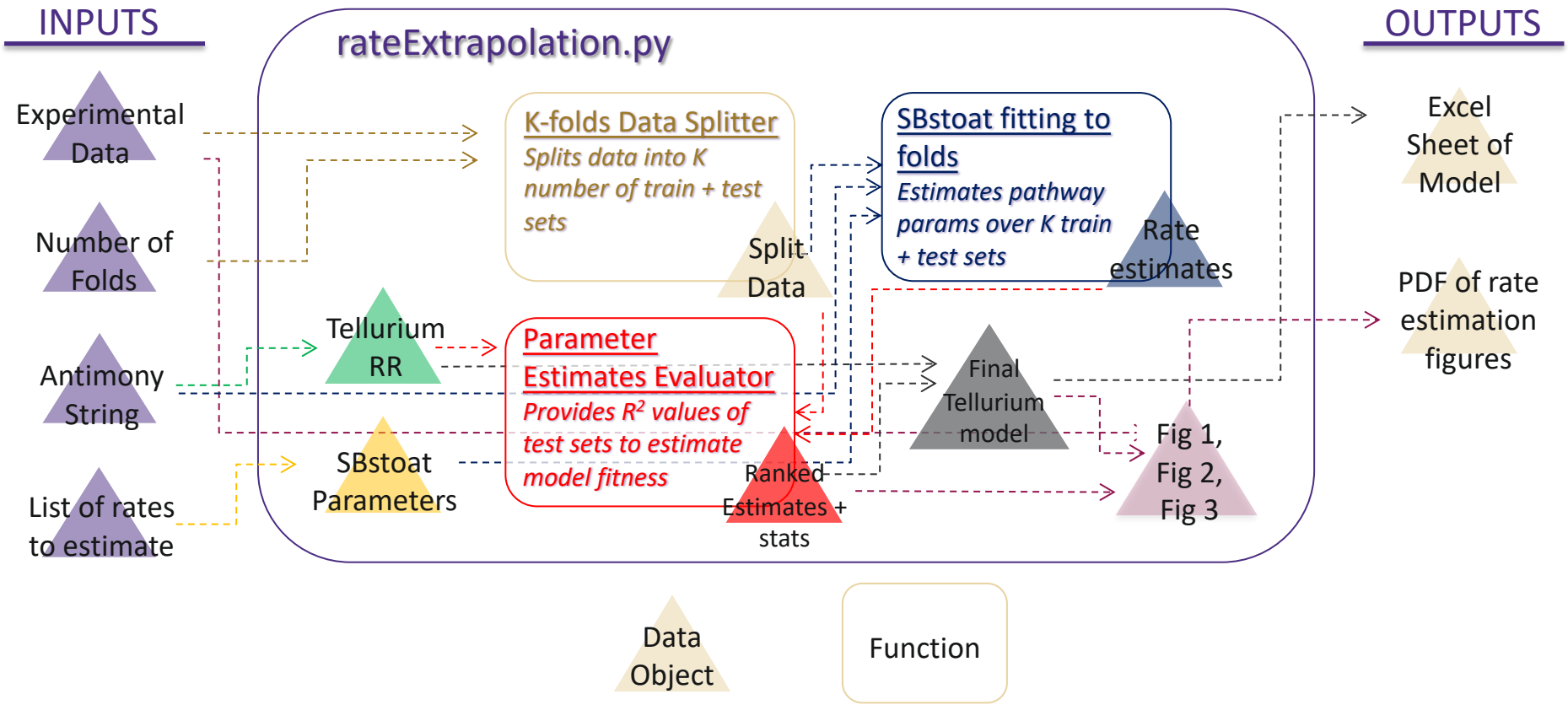
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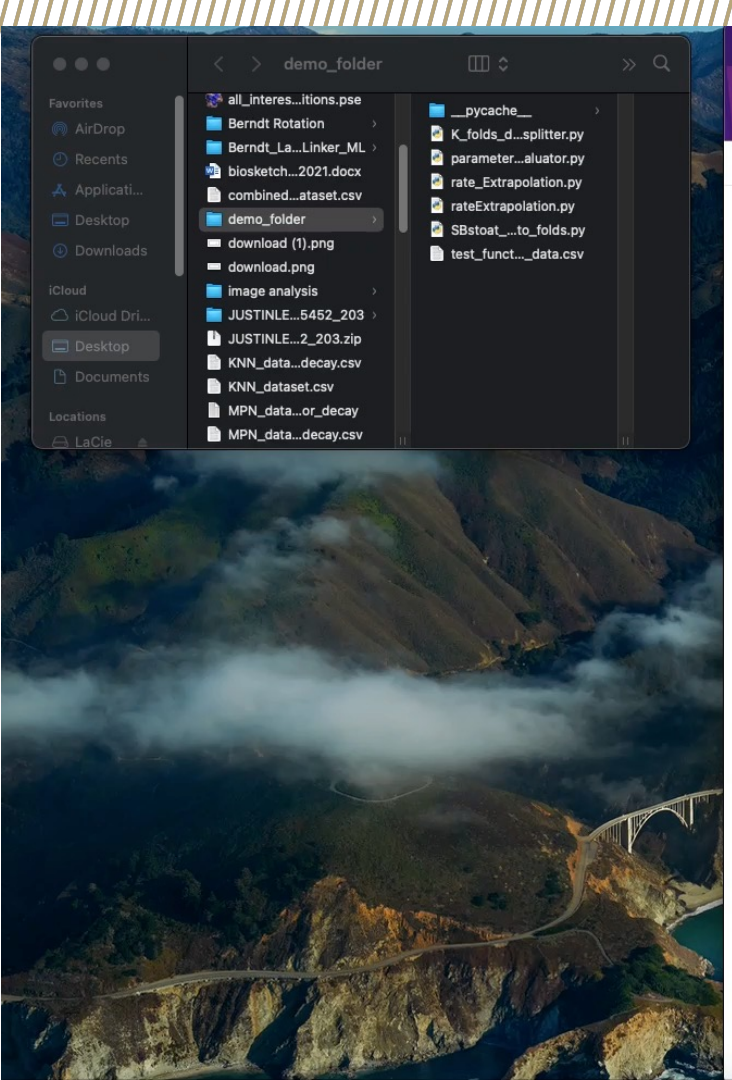
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Favorites
AirDrop
Recents
Applicati...
Desktop
Downloads
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Desktop
Documents
Locations
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Berndt_La...Linker_ML
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combined...ataset.csv
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KNN_dataset.csv
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SBstoat_...to_folds.py
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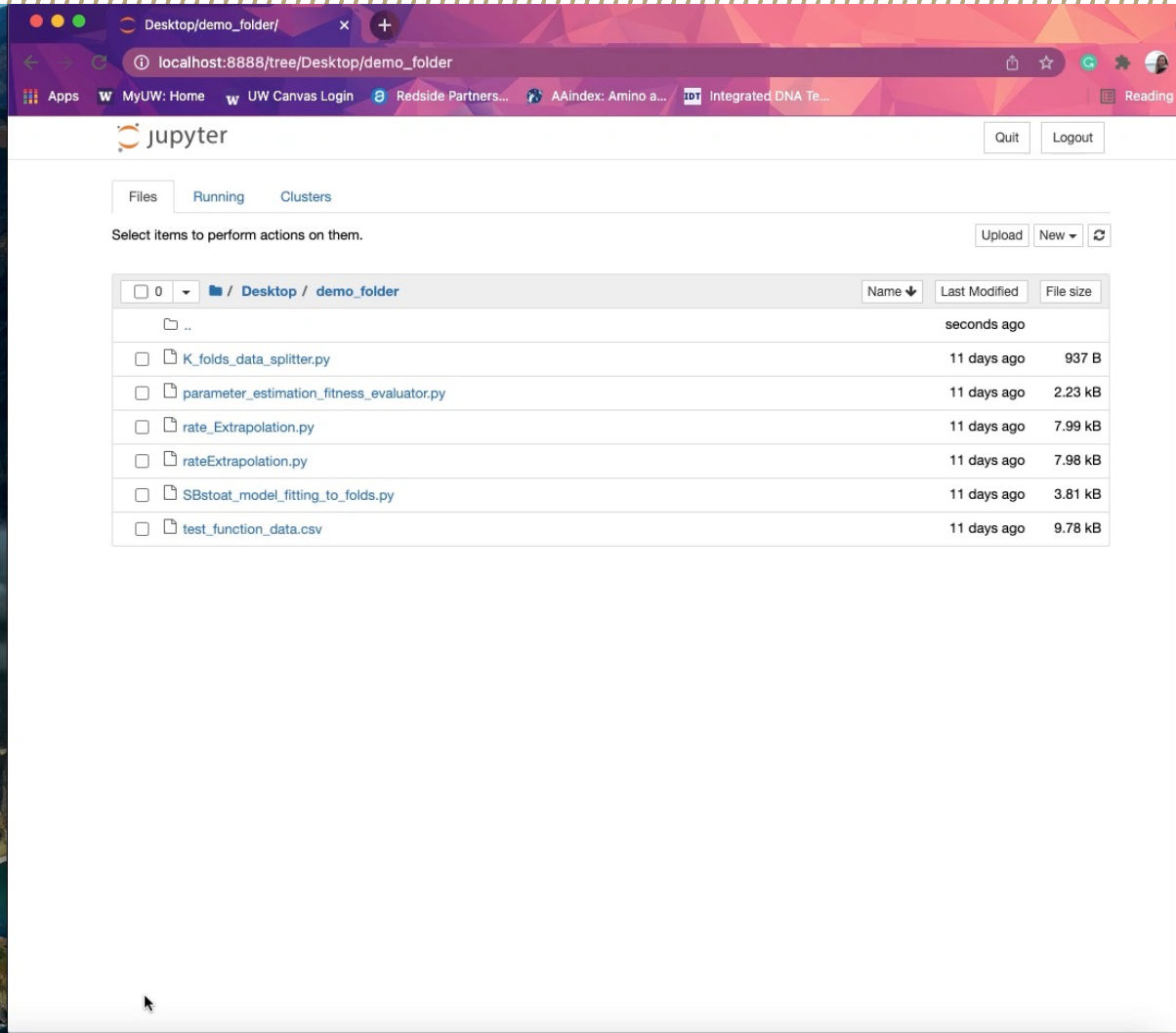
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Apps
MyUW: Home
UW Canvas Login
Redside Partners...
AAindex: Amino a...
Integrated DNA Te...
Reading
jupyter
Quit
Logout
Files
Running
Clusters
Select items to perform actions on them.
Upload
New
0
/ Desktop / demo_folder
Name
Last Modified
File size
..
seconds ago
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937 B
parameter_estimation_fitness_evaluator.py
11 days ago
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rate_Extrapolation.py
11 days ago
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7.98 kB
SBstoat_model_fitting_to_folds.py
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test_function_data.csv
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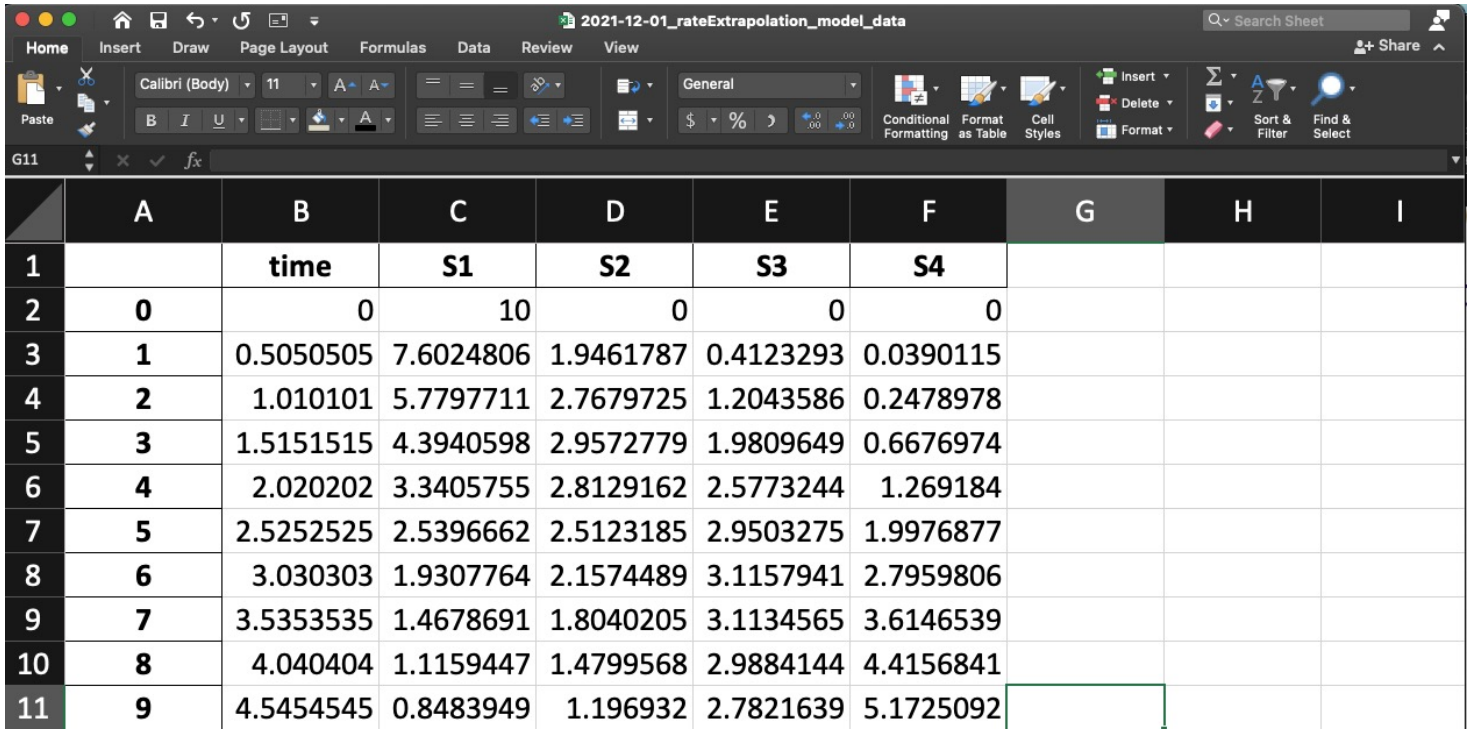
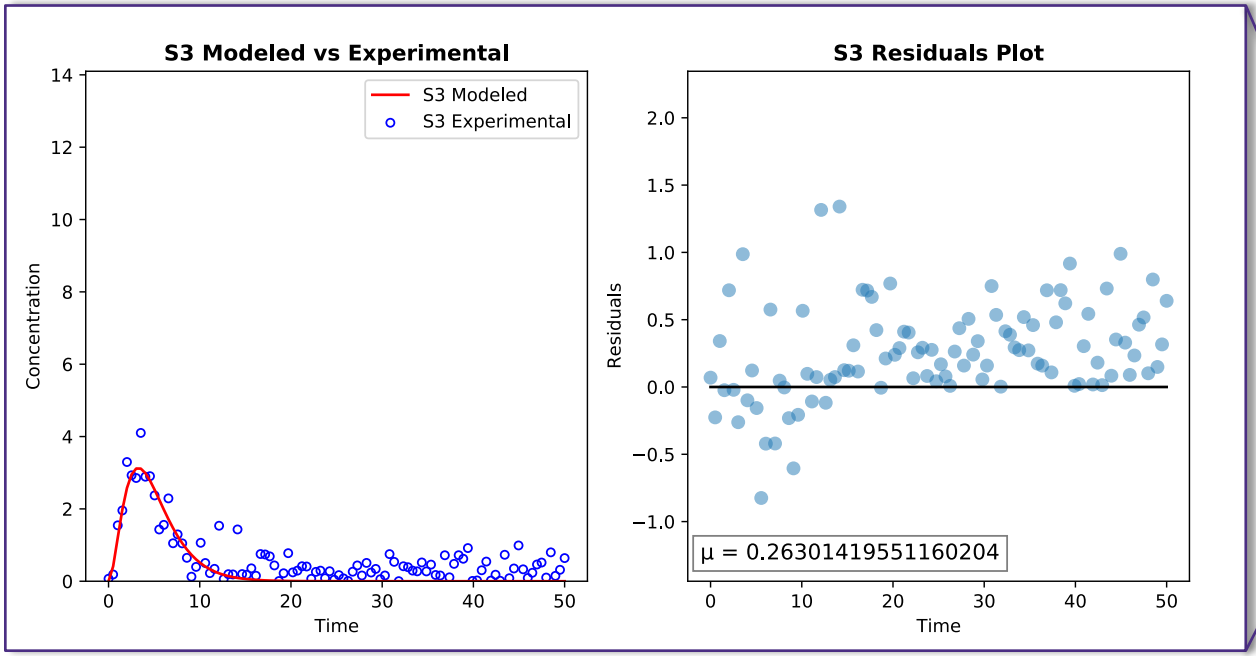
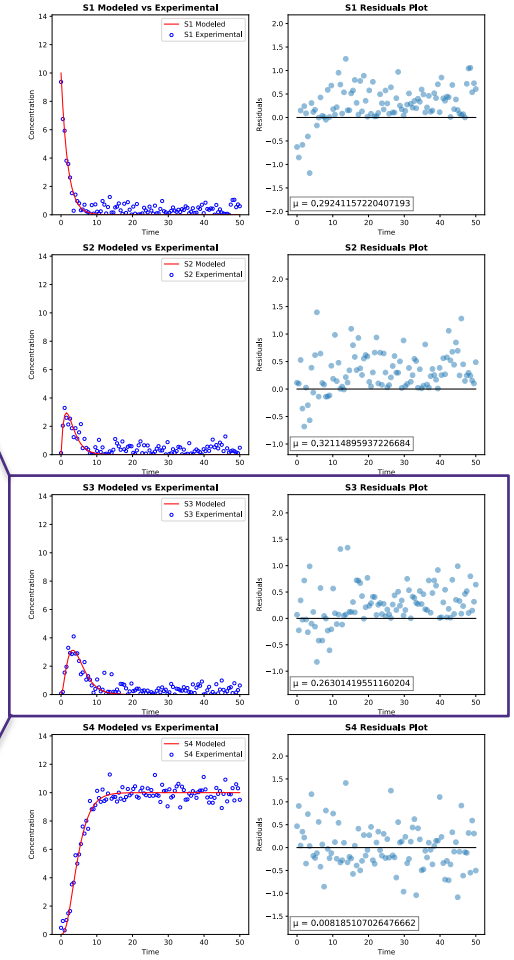
Output Excel File: *Simulated data for all substrates, not just those that were estimated*



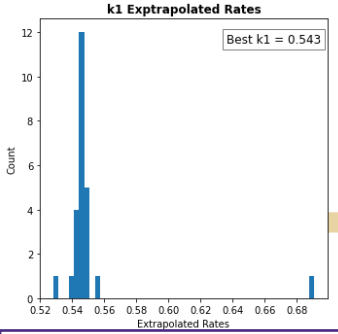
	A	B	C	D	E	F	G	H	I
1		time	S1	S2	S3	S4			
2	0	0	10	0	0	0			
3	1	0.5050505	7.6024806	1.9461787	0.4123293	0.0390115			
4	2	1.010101	5.7797711	2.7679725	1.2043586	0.2478978			
5	3	1.5151515	4.3940598	2.9572779	1.9809649	0.6676974			
6	4	2.020202	3.3405755	2.8129162	2.5773244	1.269184			
7	5	2.5252525	2.5396662	2.5123185	2.9503275	1.9976877			
8	6	3.030303	1.9307764	2.1574489	3.1157941	2.7959806			
9	7	3.5353535	1.4678691	1.8040205	3.1134565	3.6146539			
10	8	4.040404	1.1159447	1.4799568	2.9884144	4.4156841			
11	9	4.5454545	0.8483949	1.196932	2.7821639	5.1725092			

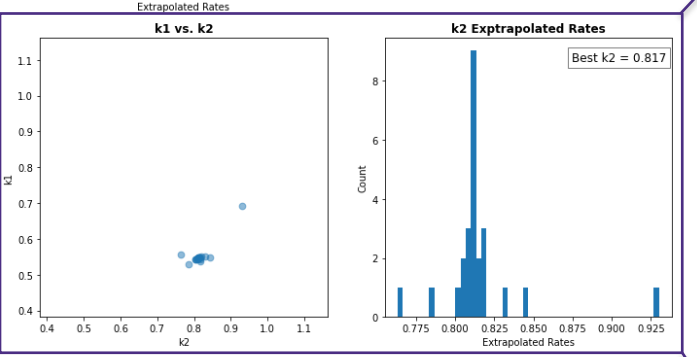
Output Figure #1: *plots of modeled vs experimental data + residuals plot*

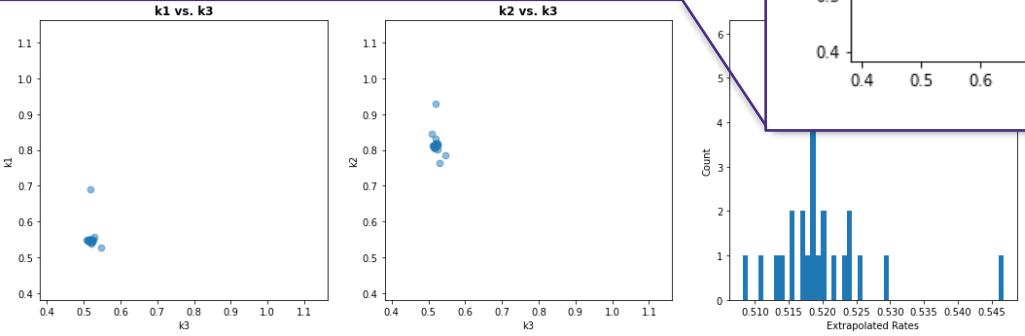


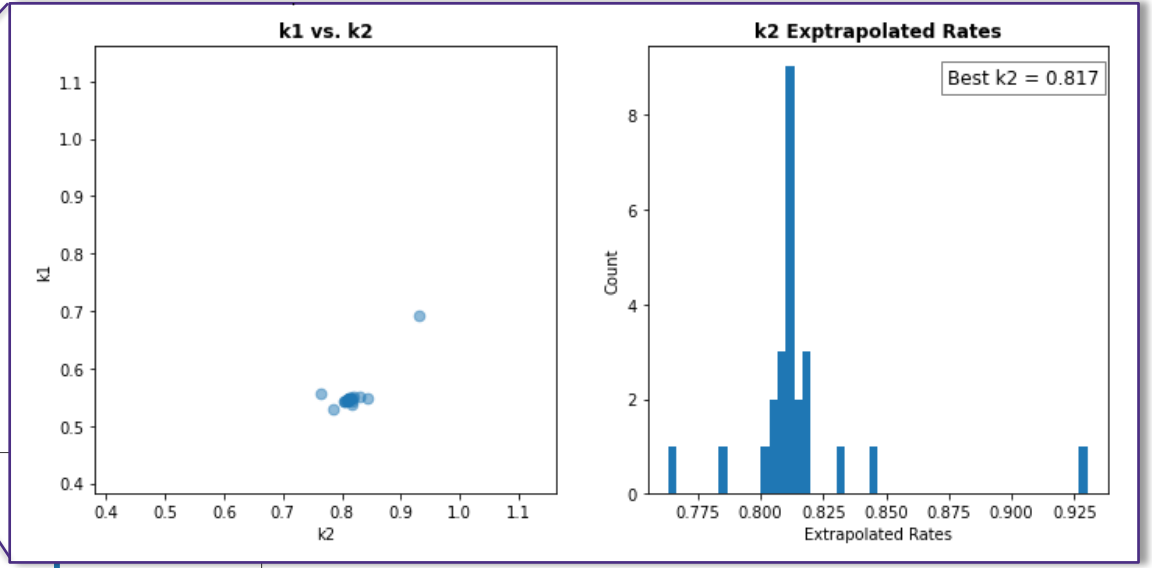


Output Figure #2: *Histograms of all estimations of rates, along with rate analysis*

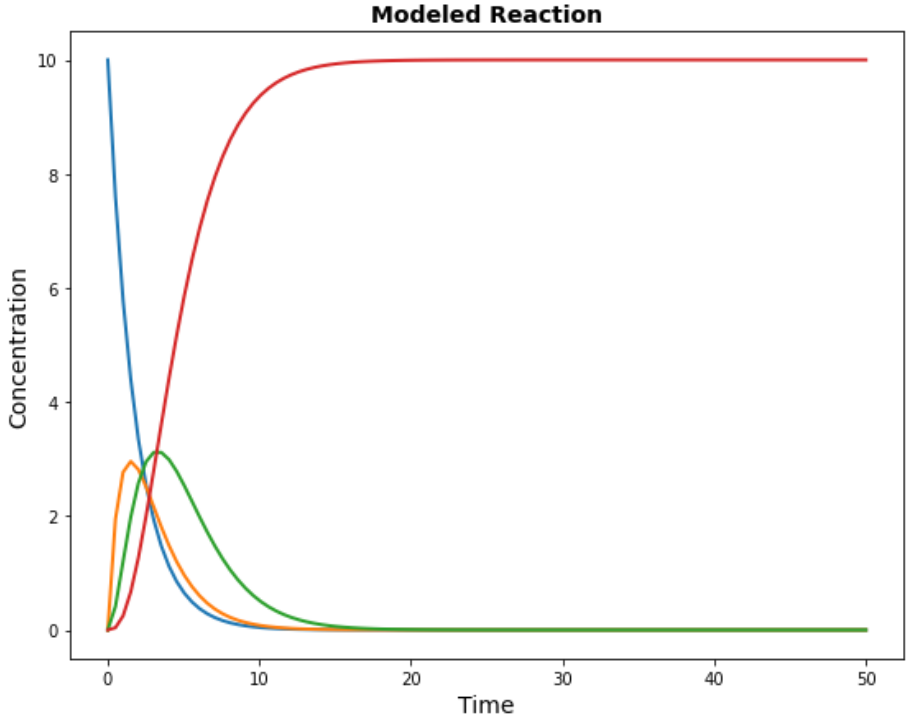


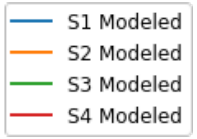






Output Figure #3: *Final summary plot of model, along with estimated parameters and statistics of model fit*





k1	0.543
k2	0.817
k3	0.518
AIC	-593.09
BIC	-581.24
Reduced χ^2	0.21
χ^2	80.68
R^2	0.988

Project Structure

TO GITHUB

https://github.com/sarahwaity/rateExtrapolation

Lessons learned and future work

- Definitely easier to start continual integration practices at the beginning of a project
  - Spent a very long time trying to get tests to pass
- Being explicit in naming not only helps future you but also limits probability of current you running into issues
- Future work:
  - Add more modularity to the function itself, (currently limited to ‘leastsquare’ extrapolation methods etc.)
  - Maybe export the PDF images into a succinct PowerPoint format
  - Be able to do all extrapolations from the command line