

Multi-variable Optimization software driven by Design of Experiments and Machine learning (**MODEM**)

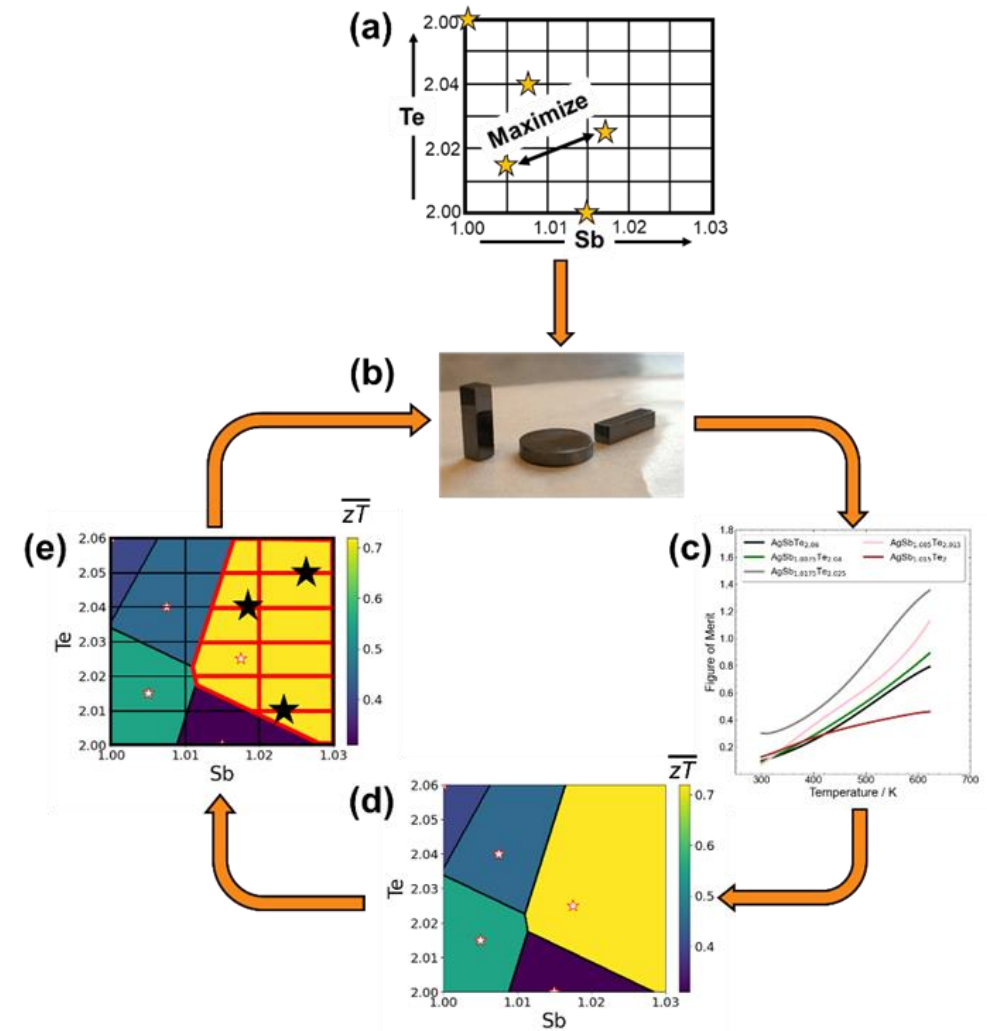
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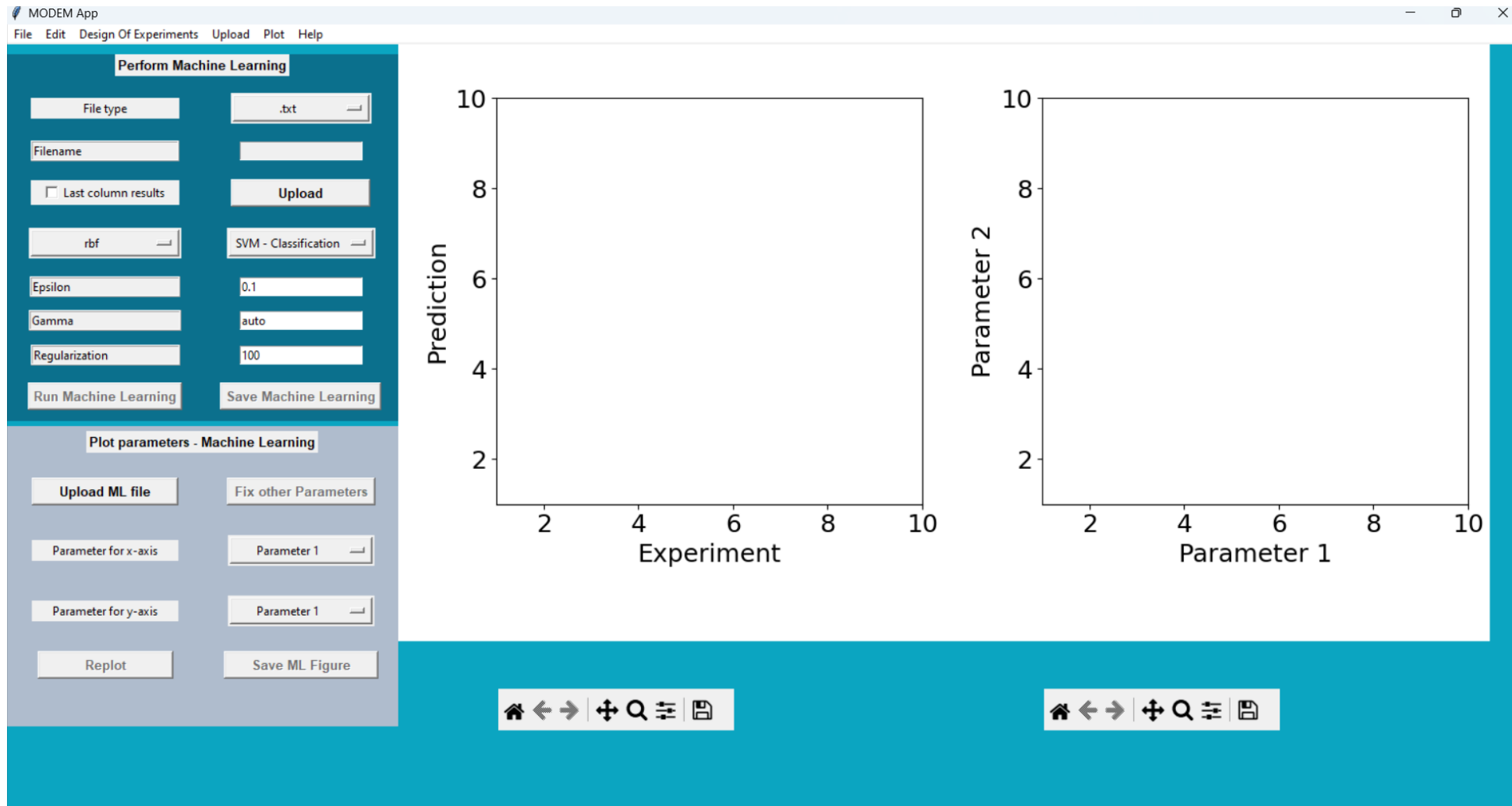
August 2024

Optimization Procedure

(a) Multiple optimal compositions were predicted using the Latin square approach in the DoE framework. (b) The samples were synthesized, and (c) the thermoelectric properties were measured. (d) A support vector classification algorithm was applied to reveal the optimum area (yellow) which is (e) a constraint for the DoE algorithm. The cycle (b-e) is repeated until the optimum composition is found. White and black stars are previous and new predicted chemical compositions, respectively, to synthesize and analyze.

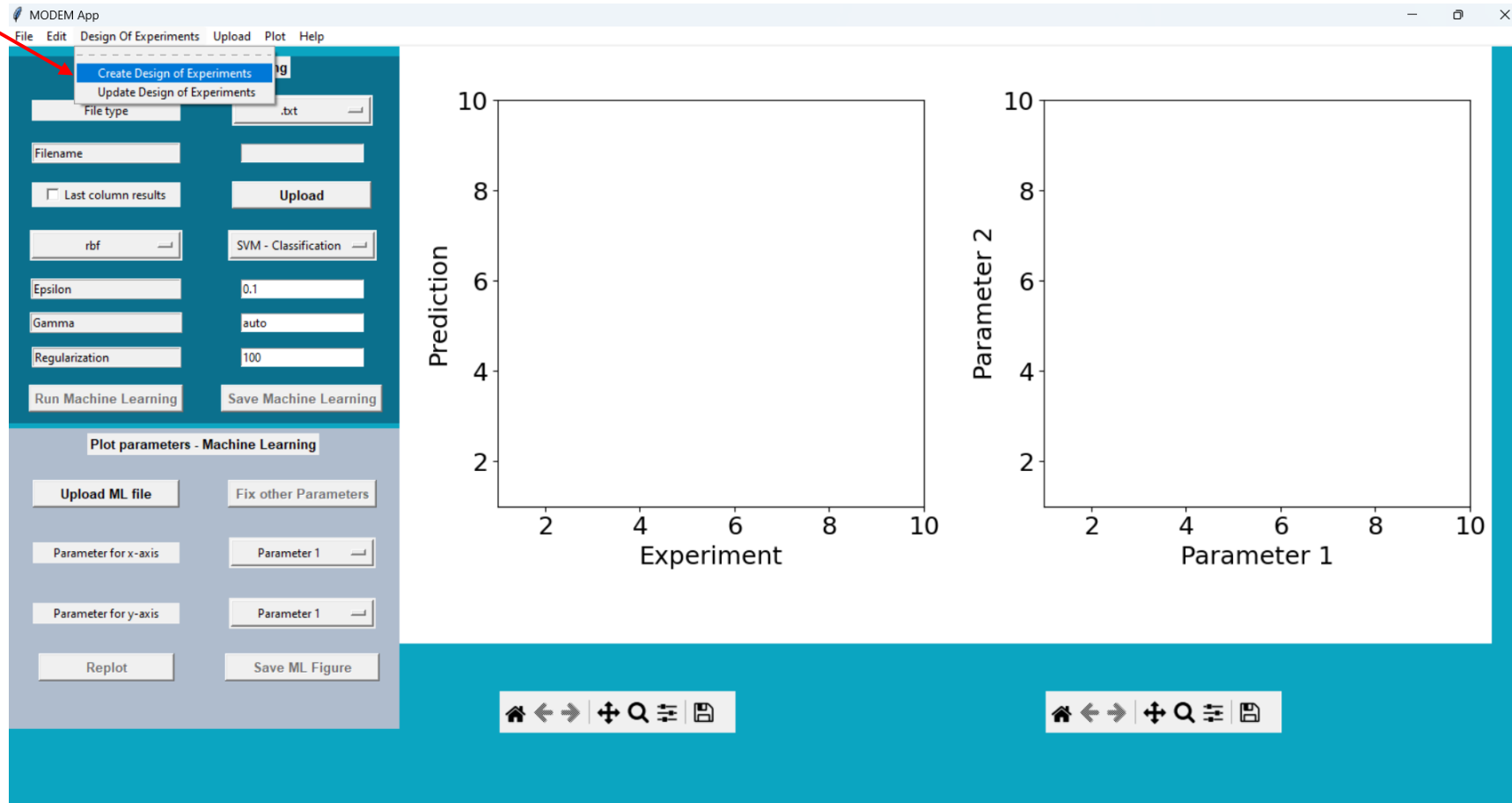


Start the Program



Initial Design of Experiments

Design of Experiments → Create Design of Experiments



Choose the Number of Variables

Number of variables → Dimensions

MODEM App

Input parameters for Design of Experiments

Dimensions of Parameters: 2

Dimensions

Close

Create the Variable Space

MODEM App

Input parameters for Design of Experiments

Dimensions of Parameters: 2

Dimension 1: Label: Parameter1, Minimum: 0.9, Maximum: 1.1, Step size: 0.01

Dimension 2: Label: Parameter2, Minimum: 0.9, Maximum: 1.1, Step size: 0.01

Number of Experiments: 6, Number of Loops: 10000, ☐ Periodic?, ☐ Center atom?, Compute

Save, Close

Names of Variables (e.g., Time)

Minimum value

Maximum value

Step size

Number of entries (Default: 2 * number of variables)

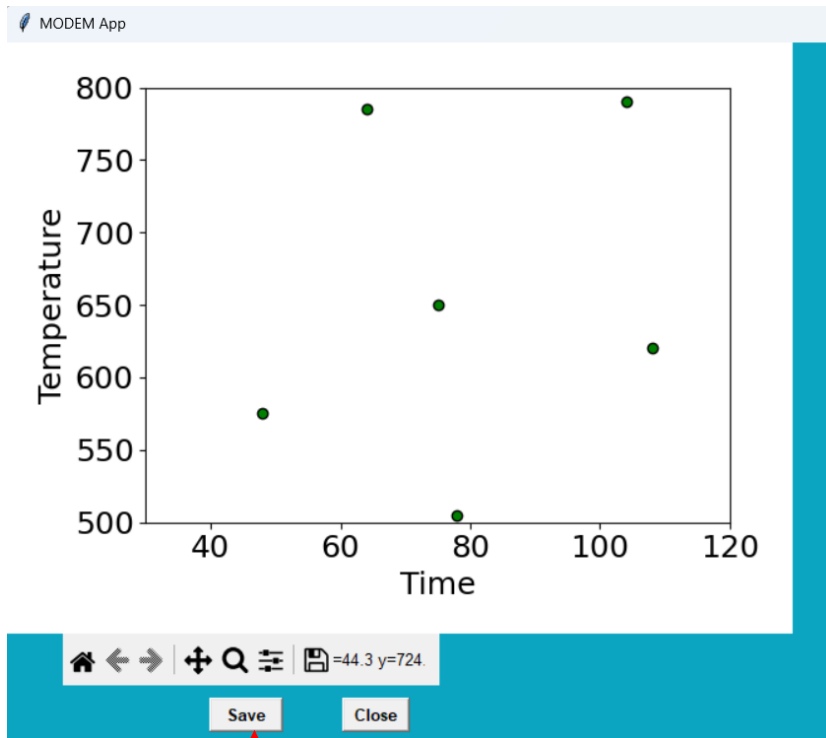
Number of Optimization Loops

Apply a Periodic Boundary Condition

Place an atom in the Center of the Variable Space

Compute

Save DoE Information



Save the DoE Figure

MODEM App

Input parameters for Design of Experiments

Dimensions of Parameters 2 Dimensions

Dimension 1 Label Time Minimum 30 Maximum 120 Step size 1

Dimension 2 Label Temperature Minimum 500 Maximum 800 Step size 5

Number of Experiments 6 Number of Loops 100000 ☐ Periodic? ☒ Center atom? Compute

Save

Close

Save the DoE Parameters as a JSON or Text Documents File
(Text Documents can also be opened in Microsoft Excel)

Upload DoE Data

Choose File Format (Text documents [.txt], JSON [.json], CSV [.csv])

The screenshot shows the MODEM App interface. The 'Perform Machine Learning' section includes a 'File type' dropdown set to '.txt', a 'Filename' input field, a 'Last column results' checkbox, an 'Upload' button, a kernel dropdown set to 'rbf', an 'SVM - Classification' dropdown, and input fields for 'Epsilon' (0.1), 'Gamma' (auto), and 'Regularization' (100). Below these are 'Run Machine Learning' and 'Save Machine Learning' buttons. The 'Plot parameters - Machine Learning' section includes an 'Upload ML file' button, a 'Fix other Parameters' button, input fields for 'Parameter for x-axis' and 'Parameter for y-axis' (both set to 'Parameter 1'), and 'Replot' and 'Save ML Figure' buttons. Two empty plots are shown on the right: 'Prediction' vs 'Experiment' and 'Parameter 2' vs 'Parameter 1'. Red arrows point from the text annotations to the file format dropdown, the 'Last column results' checkbox, and the 'Upload' button.

Check if
File includes
Results

After File
type and
Last column
results →
Upload

Fill and Save Data for Machine Learning

Insert your Measured Values/Results

MODEM App

Time	Temperature	Results
75.0	650.0	
70.0	505.0	
100.0	540.0	
90.0	790.0	
41.0	535.0	
42.0	740.0	
Parameters	Minimum	Maximum
Time	30.0	120.0
Temperature	500.0	800.0

Save data

Close

MODEM App

Time	Temperature	Results
75.0	650.0	0.7
70.0	505.0	0.6
100.0	540.0	0.75
90.0	790.0	0.9
41.0	535.0	0.3
42.0	740.0	0.8
Parameters	Minimum	Maximum
Time	30.0	120.0
Temperature	500.0	800.0

Save data

Close

Reduce Step Size

Close will give the data to
The Machine Learning
Algorithm

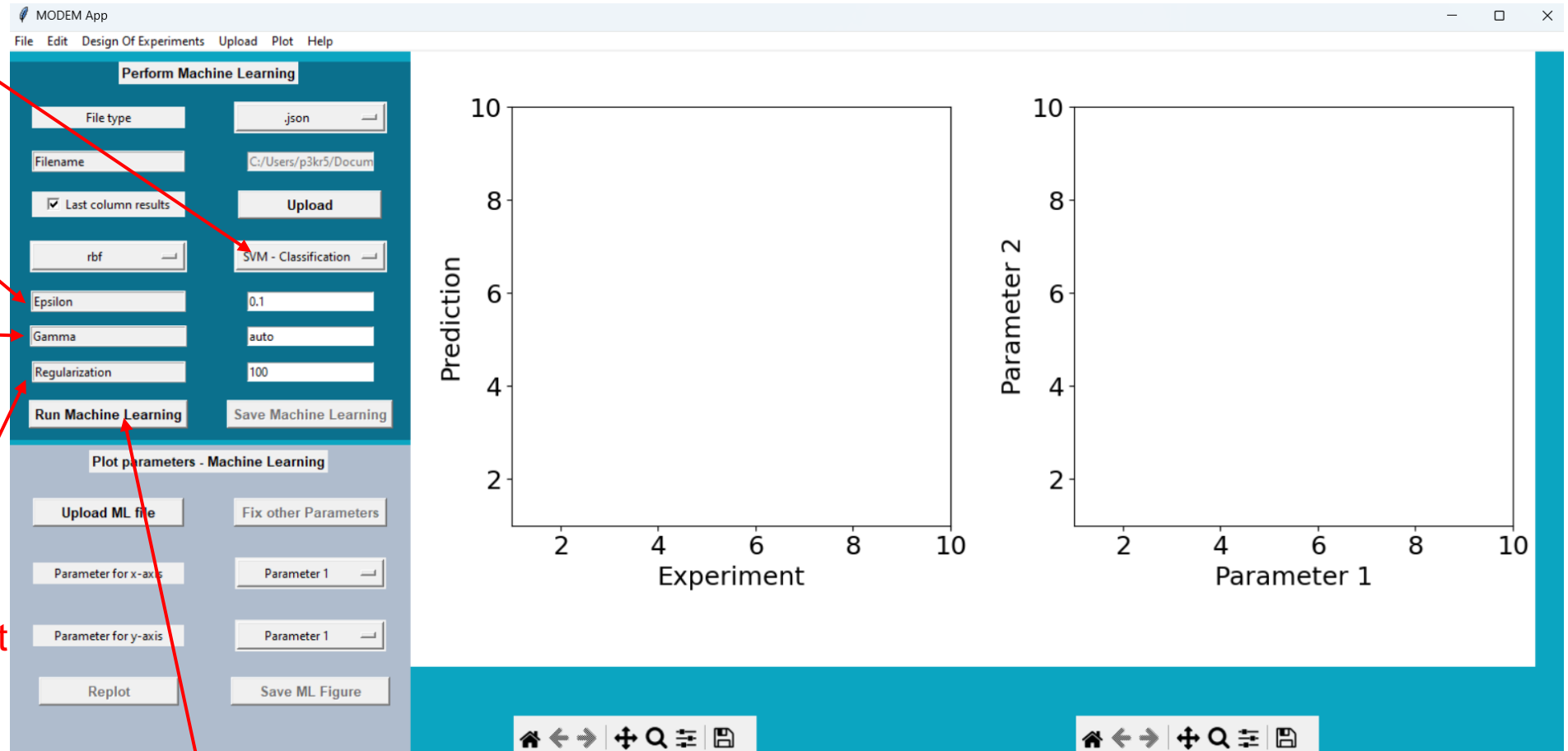
Save Data as JSON File (Faster Upload)

Run Machine Learning

Choose: **Support Vector Machine Classification** or **Support Vector Machine Regression** Algorithms

Margin of Tolerance

High Gamma: Large influence → Complex Fit
Low Gamma: Small influence → Simple Fit



Calculate Machine Learning

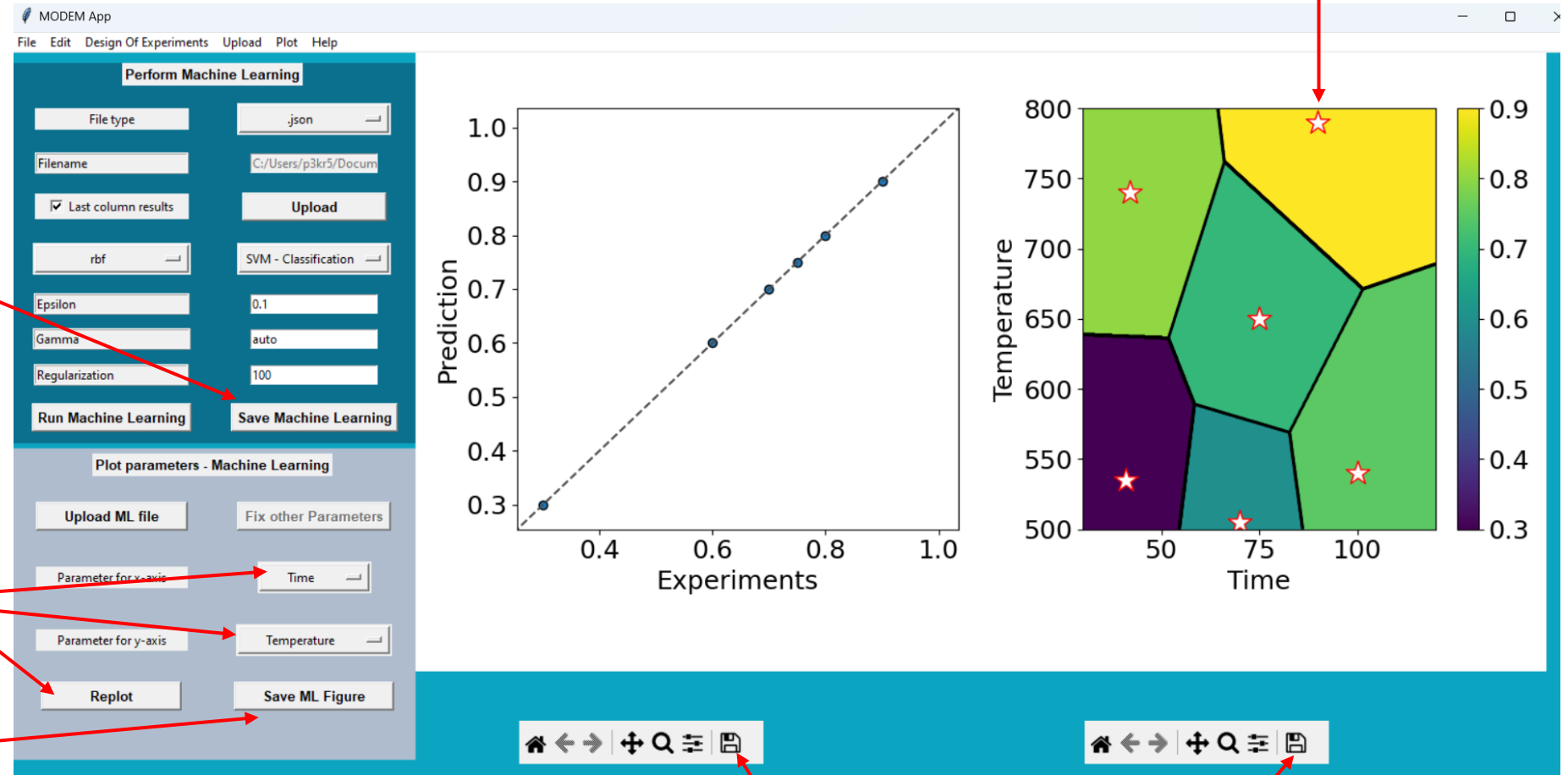
Machine Learning Plots

White Stars: Data Points
(see Slide 9)

Save Machine Learning
Data → Save Classification
for Updating Design of
Experiments

Change axes → Replot

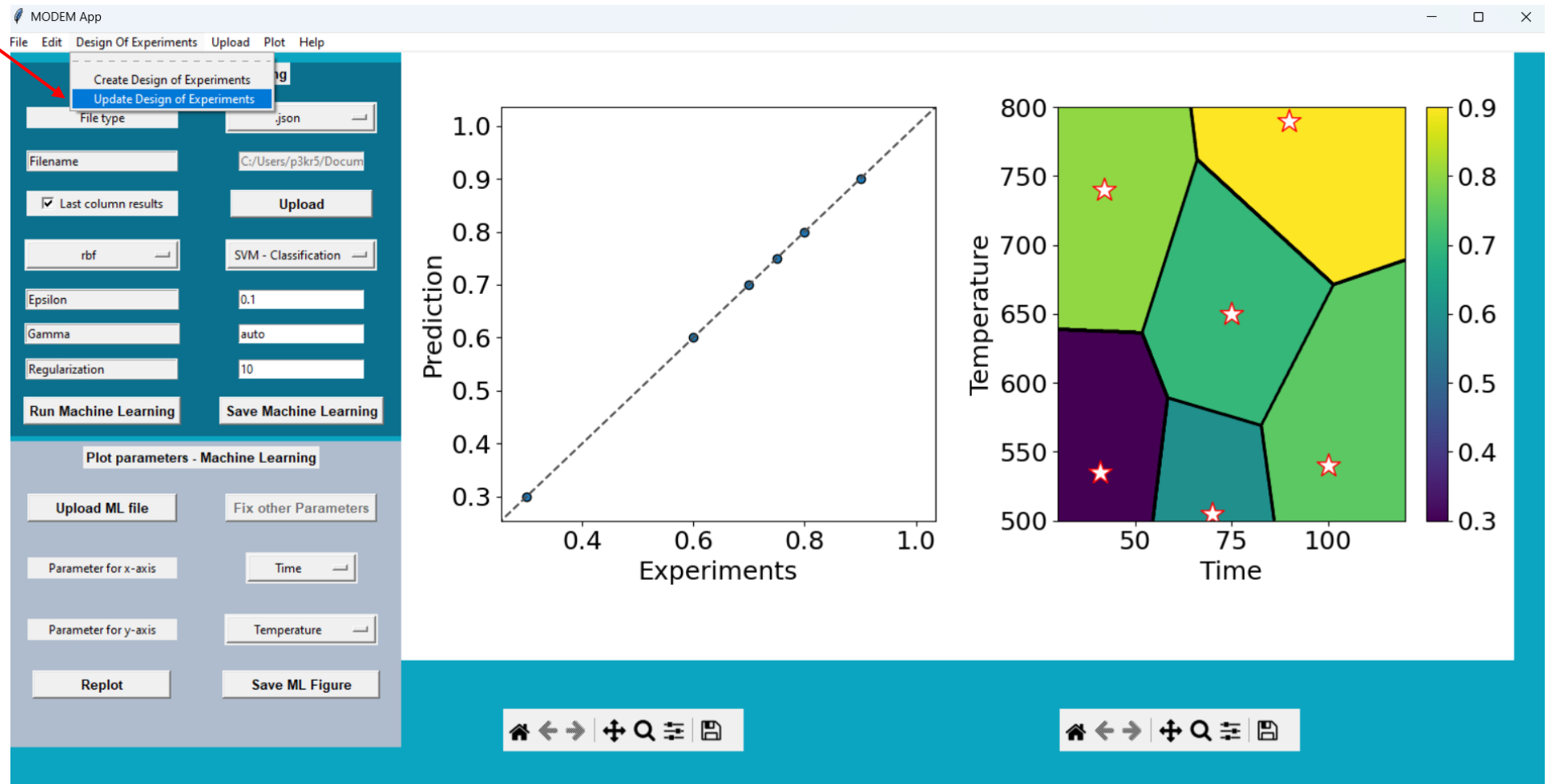
Save both Machine
Learning Figures



Save individual Machine
Learning Figures

Update Design of Experiments

Design of Experiments → Update Design of Experiments



Run Updated Classification

MODEM App Upload Classification

Input parameters for Design of Experiments

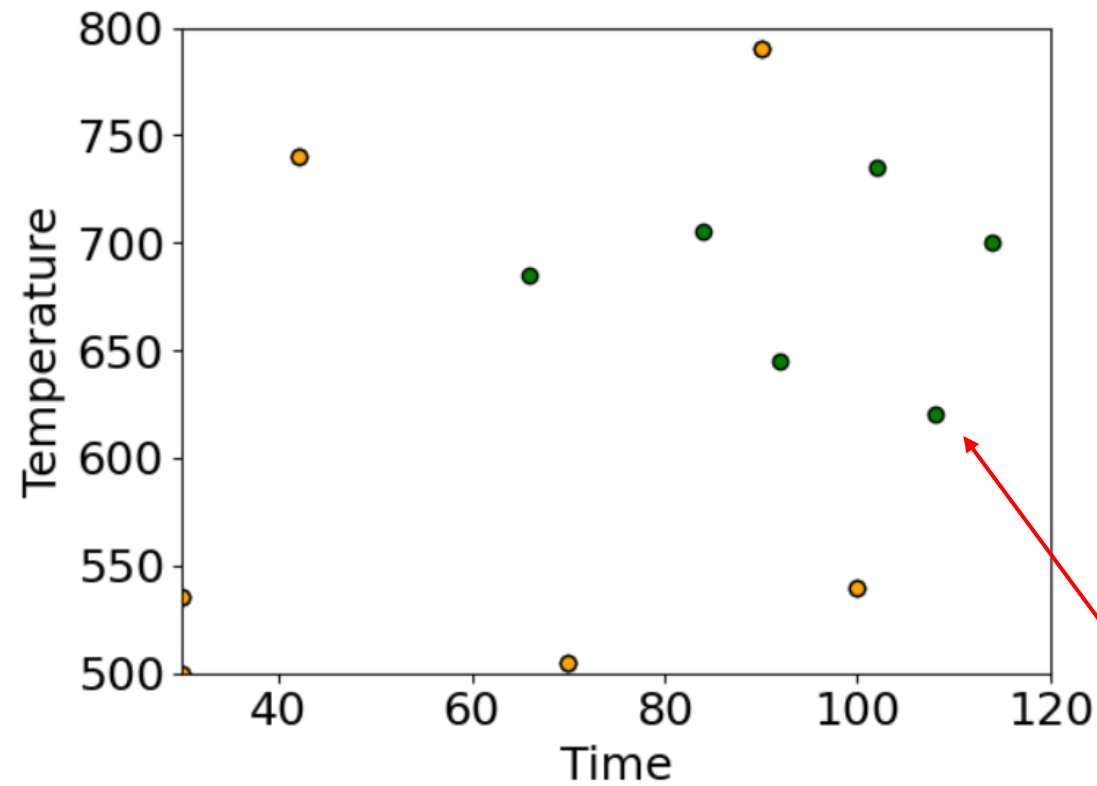
Dimensions of Parameters	2	Dimensions	Upload Classification					
Dimension 1	Label	Time	Minimum	30.0	Maximum	120.0	Step size	0.1
Dimension 2	Label	Temperature	Minimum	500.0	Maximum	800.0	Step size	0.1
Number of Experiments	6	Number of Loops	10000					
Save	Expected Value	Maximum	Desired Value	0.6				
Compute <div> Choose a value between 0.3 and 0.9 for the desired value. <div>Close</div> </div>								

Choose: - Maximum
- Minimum
- Desired Value

If desired value,
choose a value between
the given limits

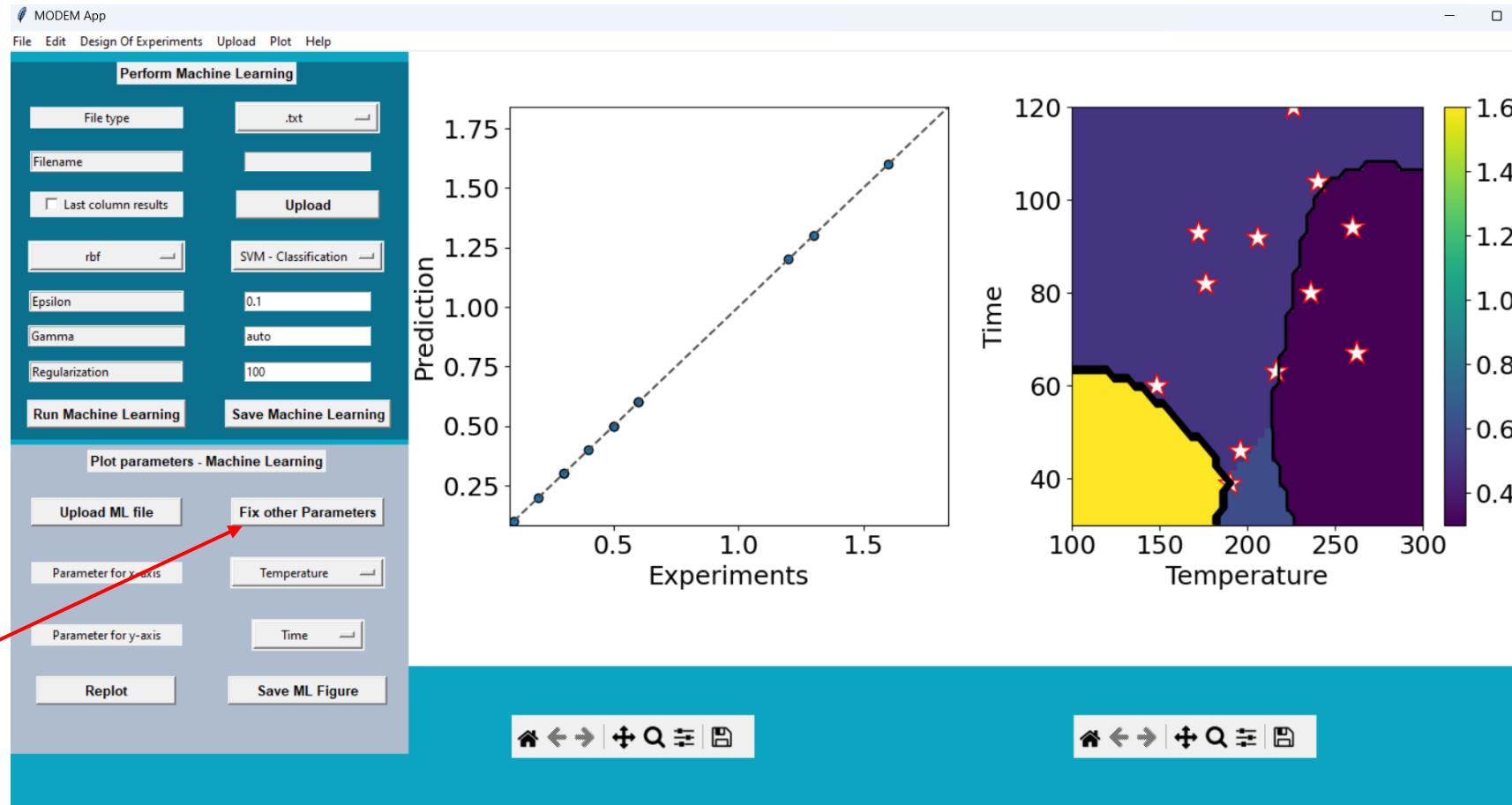
Save New DoE Data

MODEM App



Green dots = New Data

Multi-variable Machine Learning



Fix other
Parameters

Plot Heatmap of Desired Plane

If Predicted value is checked,
Choose between maximum,
Minimum, or Desired value

Change between Predicted value
and Step(s)

MODEM App

Input parameters to fixed the remaining axis (more than two variables)

Choose the maximum, minimum, or a desired predicted value

☒ Predicted value

☐ Maximum

☐ Desired Value

0.1

Plot

Choose the step(s) for the remaining variables

☐ Step(s)

Axis 3 Doping A 0.800

Axis 4 Doping B 0.000

Change

Close

Plot to update the
ML figure

Choose a desired
Value from list (classification)
or set it (regression)

If Step(s) is checked,
change the values for the other axes

Questions?

If you have any questions, please send an email to:
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