

Workshop – Prediction Analysis, Buckling

AN MSC NASTRAN MACHINE LEARNING WEB APP TUTORIAL

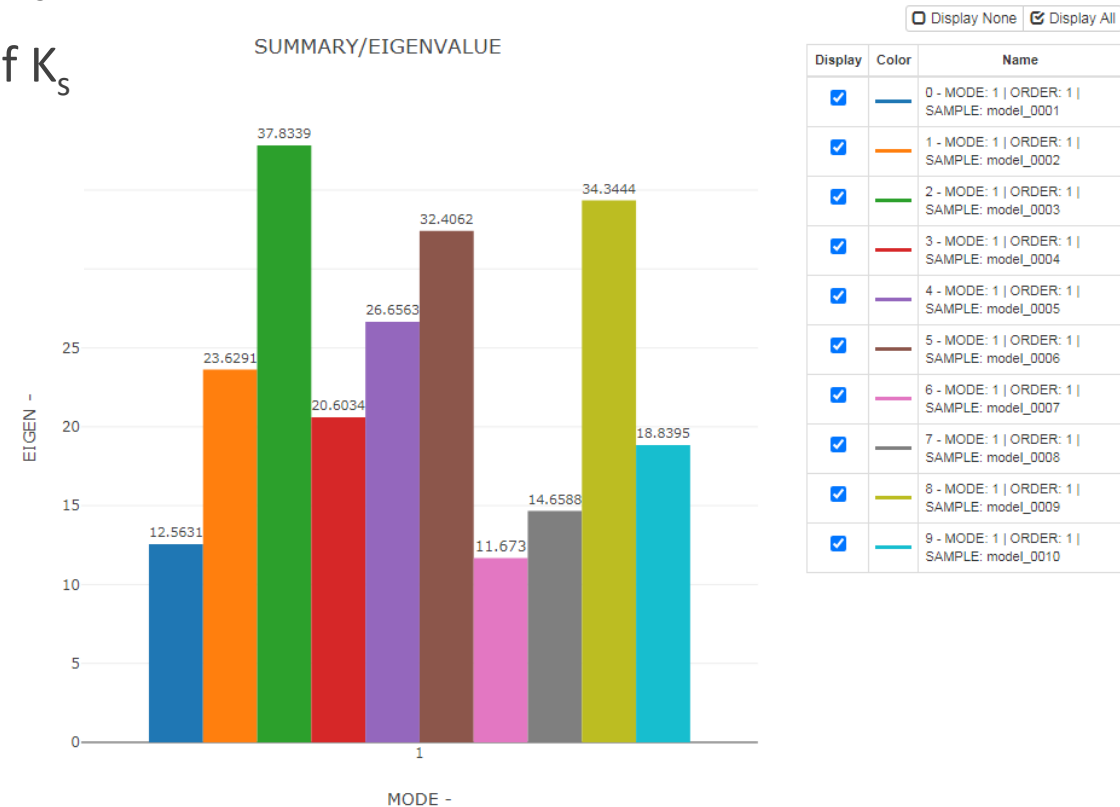
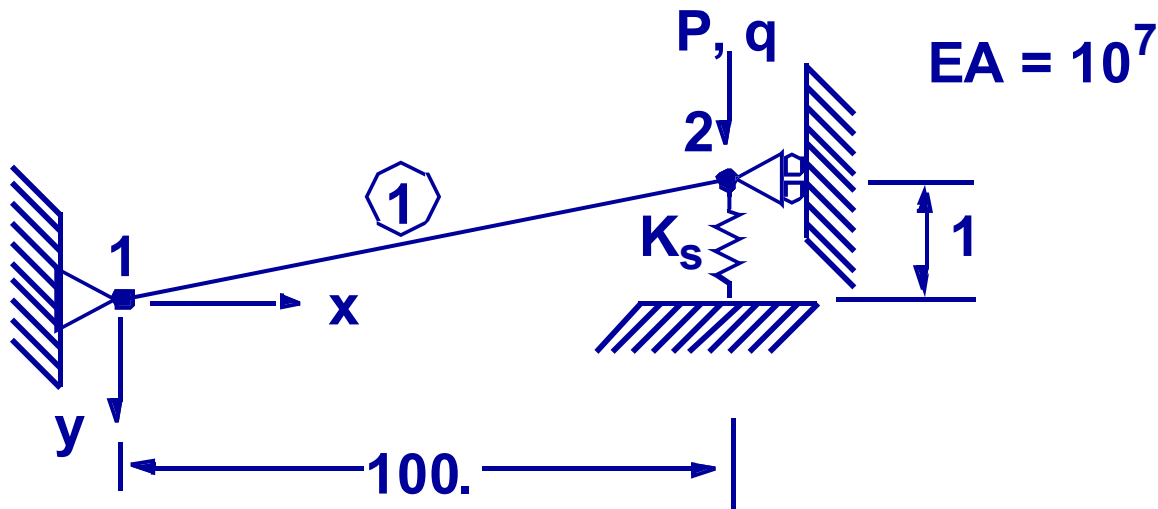
Goal: Prediction Analysis

This tutorial consists of multiple parts

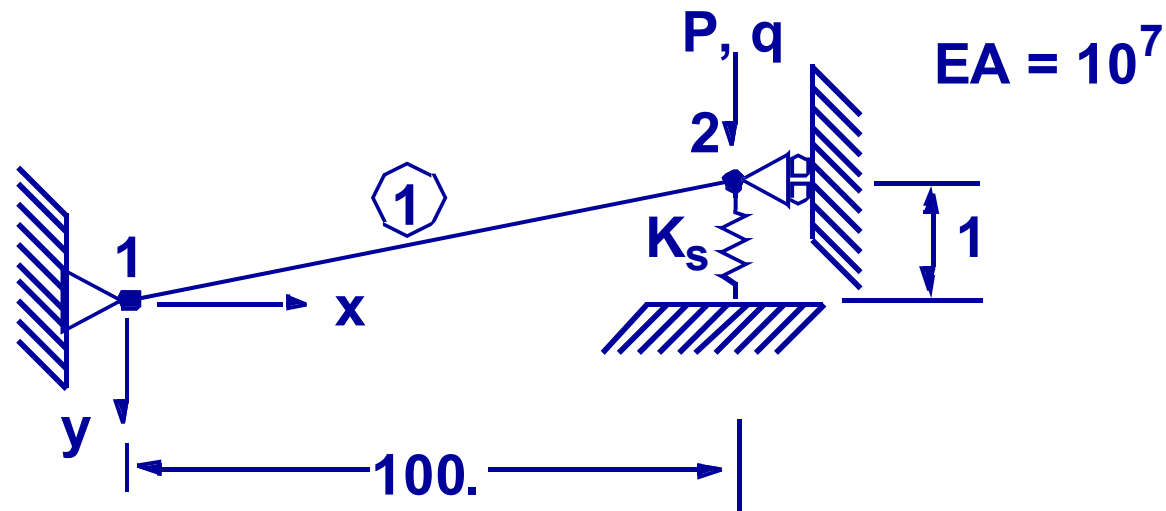
1. Configuring The Problem Statement
 - In this tutorial, we configure the parameters and the responses to monitor.
2. Configuring Multiple Batch Runs
 - This section discusses how to configure and execute multiple MSC Nastran runs.
3. Performing Predictions
 - Gaussian process (GP) regression is used to train a surrogate model and perform predictions.
 - The prediction performance of the surrogate model is evaluated.
4. Creating Plots with the HDF5 Explorer
 - The HDF5 Explorer web app is used to create Eigenvalue vs. Mode Number plots.

Details of the Structural Model

1. Perform a buckling analysis for different values of K_s
2. Monitor the eigenvalue response for each value of K_s



Details of the Structural Model



Problem Statement

Design Variables

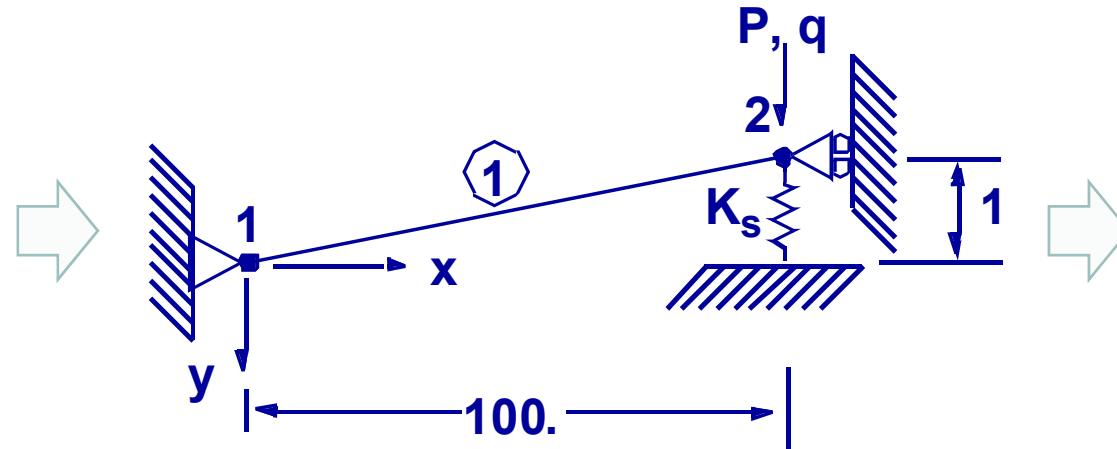
x1: K of PELAS 20

Note that K is displayed as K_s in the figure

$$.1 < x1 < 10.0$$

Samples

- Batch set 1 – 10 run LHS Design
- Batch set 2 – 20 run LHS Design



Monitored Responses

r0: Eigenvalue of Mode 1

Contact me

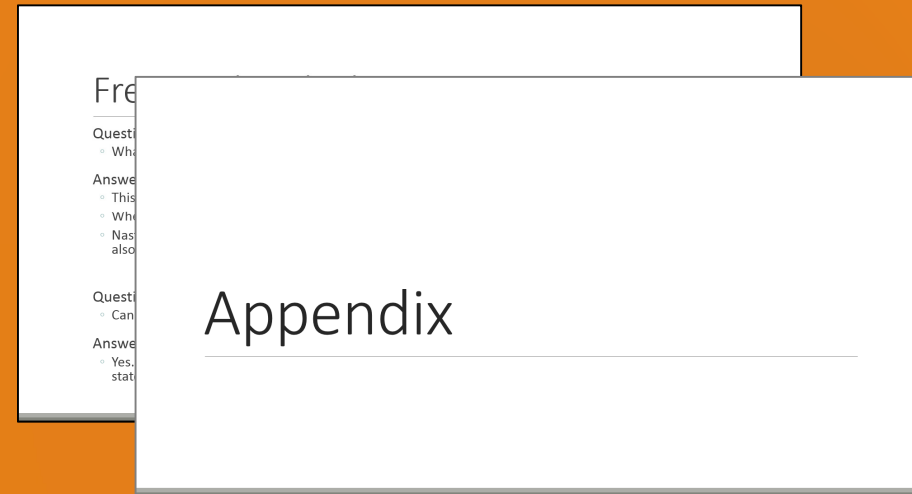
- Nastran SOL 200 training
- Nastran SOL 200 questions
- Structural or mechanical optimization questions
- Access to the SOL 200 Web App

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More Information Available in the Appendix

The Appendix includes information regarding the following:

- How to import and edit previous files
- What is Gaussian Process Regression?



Tutorial

Tutorial Overview

1. Start with a .bdf or .dat file
2. Use the Machine Learning web app to:
 1. Configure the problem statement
 2. Configure multiple batch runs
3. Use the Prediction Analysis web app to:
 1. Perform predictions
4. Use the HDF5 Explorer to:
 1. Create plots

Special Topics Covered

Training Data – The training data consists of the parameter inputs and respective output responses for multiple MSC Nastran runs. This tutorial describes how to configure multiple MSC Nastran runs, each with different parameter inputs, and how to monitor each response.

Gaussian process regression – This tutorial describes the procedure to use Gaussian process regression to train a surrogate model and make predictions.

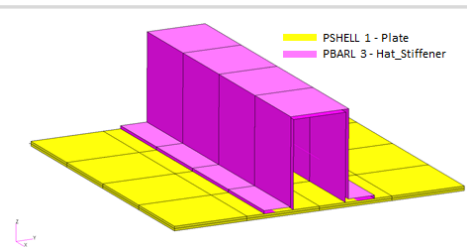
Automatic Response Extraction – Often responses are manually or automatically extracted from the F06 file. This becomes challenging when extracting responses from multiple F06 files. This tutorial highlights the web app's ability to automatically extract responses from multiple H5 files with minimal user effort.

SOL 200 Web App Capabilities

Benefits

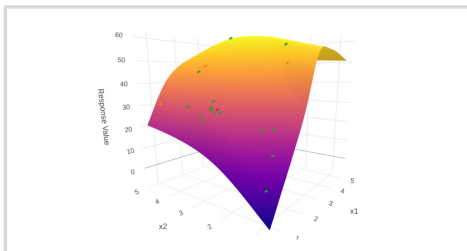
- 200+ error validations (real time)
- Web browser accessible
- Automated creation of entries (real time)
- Automatic post-processing
- 76 tutorials

Capabilities



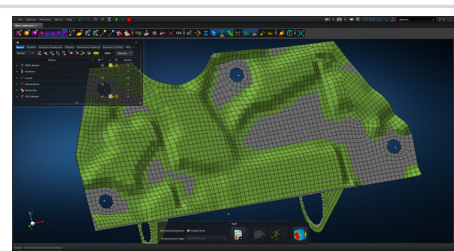
Web Apps for SOL 200

Pre/post for MSC Nastran SOL 200.
Support for size, topology, topometry, topography and multi-model.



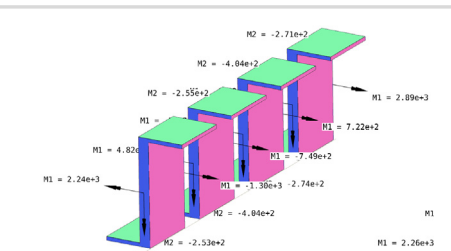
Machine Learning Web App

Bayesian Optimization for nonlinear response optimization (SOL 400)



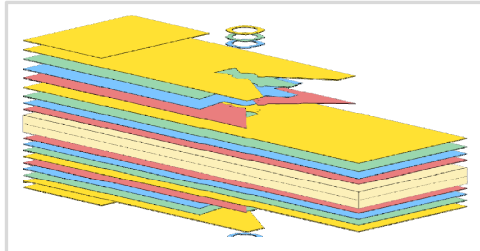
MSC Apex Post Processing Support

View the newly optimized model after an optimization



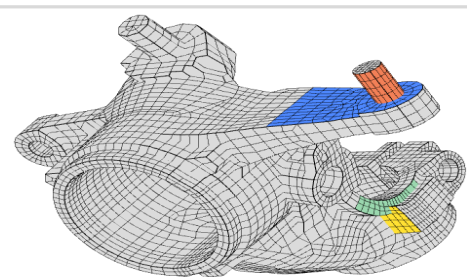
Beams Viewer Web App

Post process 1D element forces, including shear forces, moments, torque and axial forces



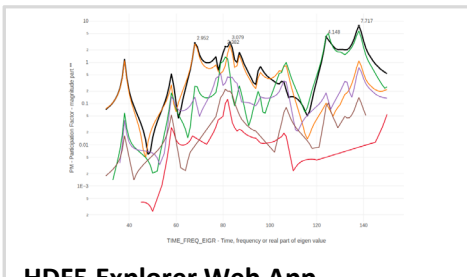
Ply Shape Optimization Web App

Spread plies optimally and generate new PCOMPG entries



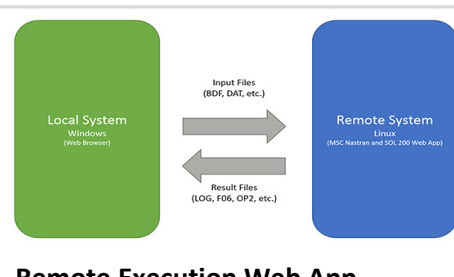
Shape Optimization Web App

Use a web application to configure and perform shape optimization.



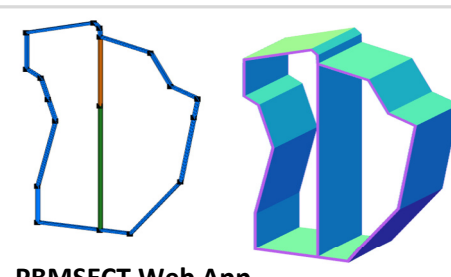
HDF5 Explorer Web App

Create XY plots using data from the H5 file



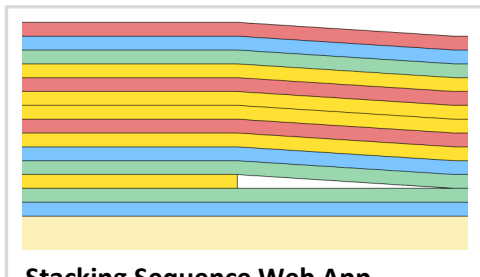
Remote Execution Web App

Run MSC Nastran jobs on remote Linux or Windows systems available on the local network



PBMSECT Web App

Generate PBMSECT and PBRSECT entries graphically



Stacking Sequence Web App

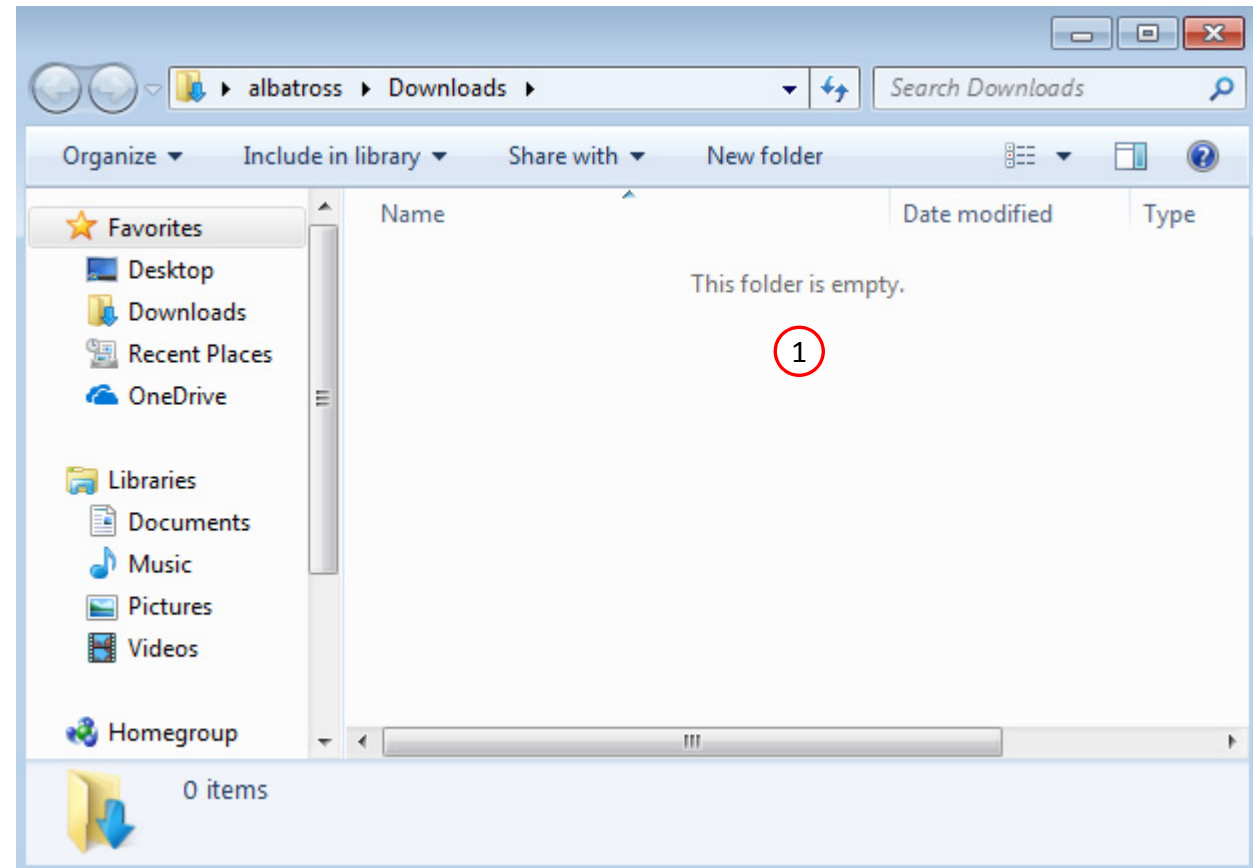
Optimize the stacking sequence of composite laminate plies

Configuring The Problem Statement

Before Starting

1. Ensure the Downloads directory is empty in order to prevent confusion with other files

- Throughout this workshop, you will be working with multiple file types and directories such as:
 - .bdf/.dat
 - nastran_working_directory
 - .f06, .log, .pch, .h5, etc.
- To minimize confusion with files and folders, it is encouraged to start with a clean directory.



Go to the User's Guide

1. Click on the indicated link

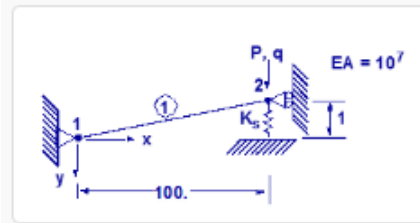
- The necessary BDF files for this tutorial are available in the Tutorials section of the User's Guide.



Obtain Starting Files

1. Find the indicated example
2. Click Link
3. The starting file has been downloaded

- When starting the procedure, all the necessary BDF, or DAT, files must be collected and uploaded together. Relevant INCLUDE files must also be collected and uploaded.



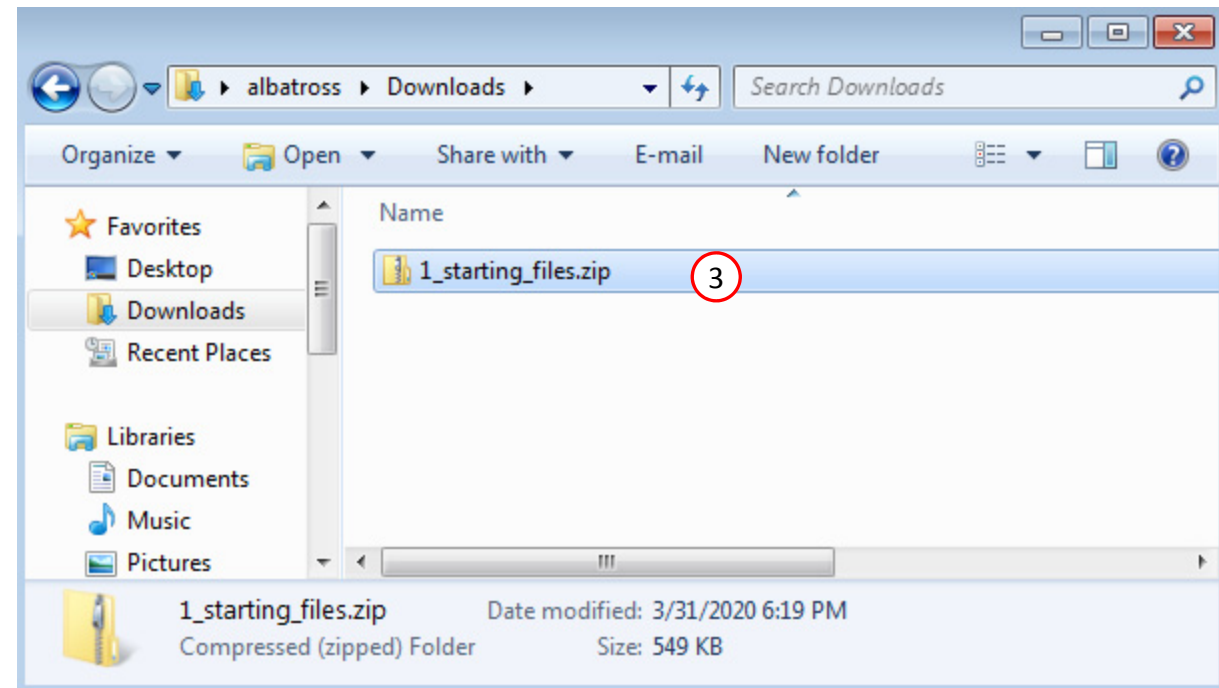
Prediction Analysis, Buckling ①

Consider a linear buckling analysis. The parameter allowed to vary is a spring constant. The response of interest is the buckling load factor.

This tutorial describes how to configure multiple MSC Nastran runs to generate training data. Gaussian process regression is used to train a surrogate model and make predictions. The prediction performance of the surrogate model is also evaluated.

Starting Files [Link](#)

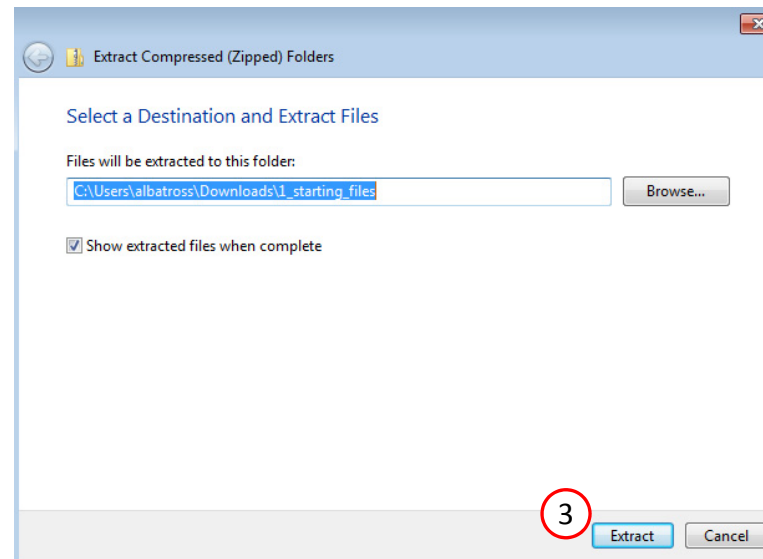
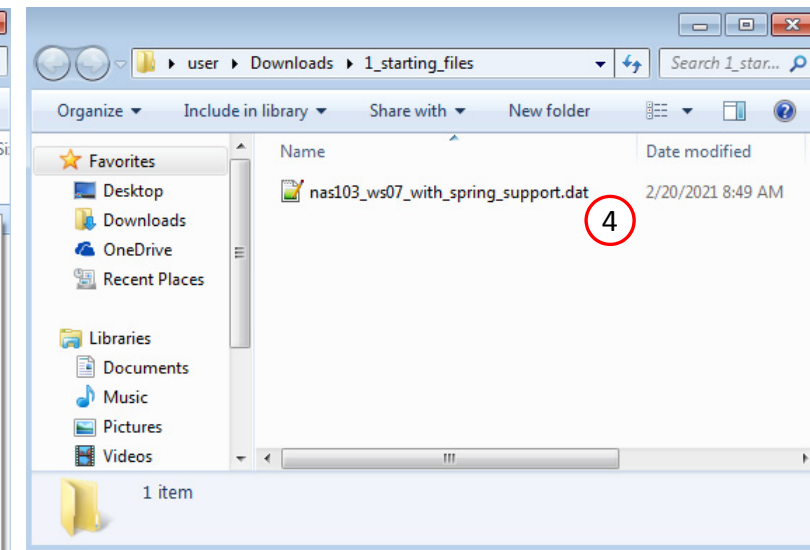
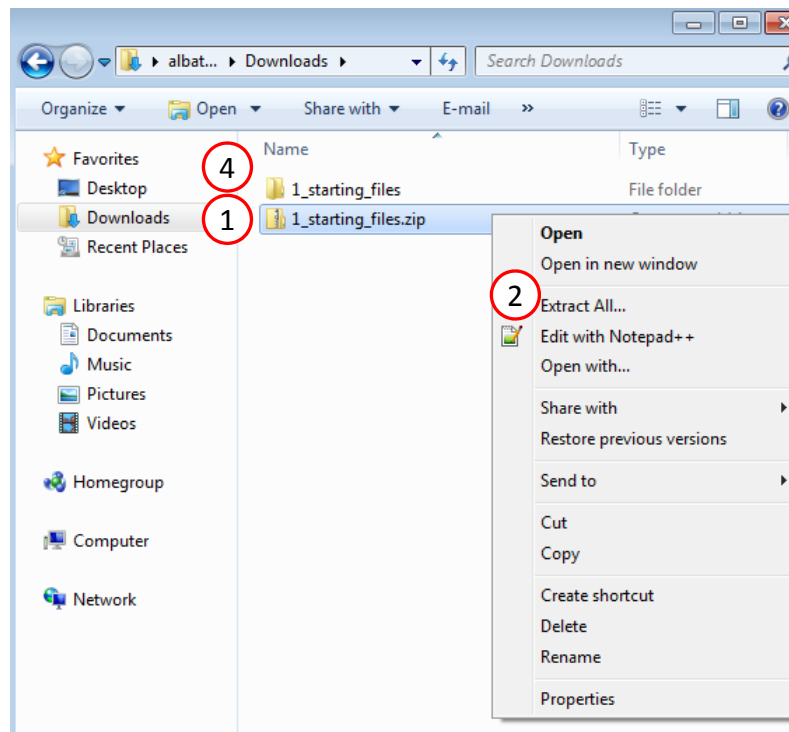
Solution BDF Files: [Link](#)



Obtain Starting Files

1. Right click on the zip file
2. Select Extract All...
3. Click Extract
4. The starting files are now available in a folder

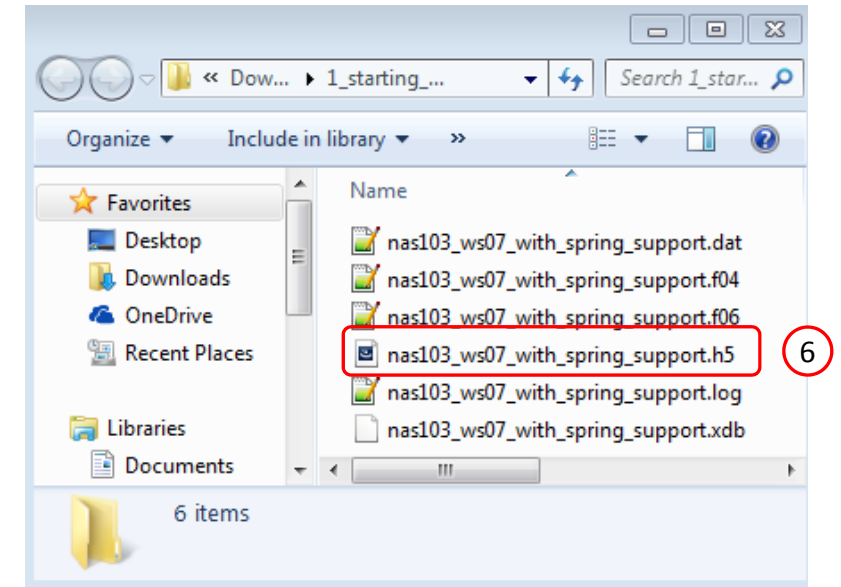
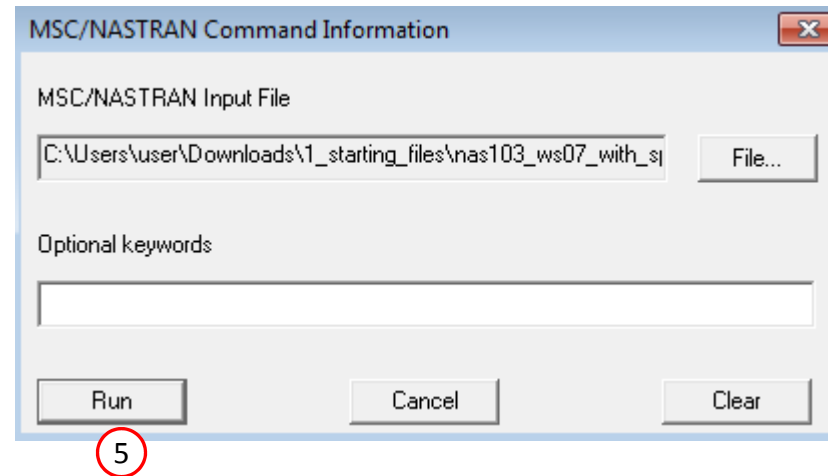
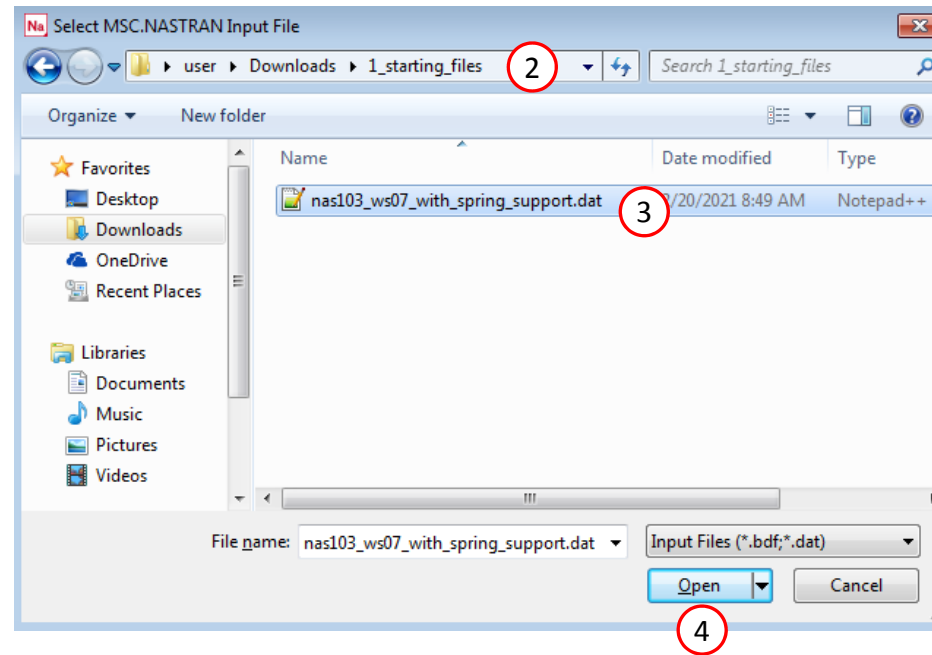
- The starting files for this tutorial are contained in a ZIP file and must be extracted as shown.



Create the Starting H5 File

A starting H5 file must be created. This H5 file will be used to configure the responses later on.

1. Double click the MSC Nastran desktop shortcut
2. Navigate to the directory named 1_starting_files
3. Select the indicated file
4. Click Open
5. Click Run
6. The starting H5 file is created



Use the same MSC Nastran version throughout this exercise

The following applies if you have multiple versions of MSC Nastran installed.

To ensure compatibility, use the same MSC Nastran version throughout this exercise. For example, scenario 1 is OK but scenario 2 is NOT OK.

- Scenario 1 - OK
 - MSC Nastran 2021 is used to create the starting H5 file.
 - MSC Nastran 2021 is used for each run during Machine Learning or Parameter study.
- Scenario 2 – NOT OK
 - MSC Nastran 2018.2 is used to create the starting H5 file.
 - MSC Nastran 2021 is used for each run during Machine Learning or Parameter study.

Using the same MSC Nastran version is critical for consistent response extraction from the H5 file. A response configured for Nastran version X may not match in Nastran version Y, which leads to unsuccessful response extraction from the H5 files. The goal is to make sure all H5 files generated are from the same MSC Nastran version.

Open the Correct Page

1. Click on the indicated link

- MSC Nastran can perform many optimization types. The SOL 200 Web App includes dedicated web apps for the following:
 - Optimization for SOL 200 (Size, Topology, Topometry, Topography, Local Optimization, Sensitivity Analysis and Global Optimization)
 - Multi Model Optimization
 - Machine Learning
- The web app also features the HDF5 Explorer, a web application to extract results from the H5 file type.

The screenshot displays the SOL 200 Web App interface. At the top, the title "SOL 200 Web App" is centered, followed by the instruction "Select a web app to begin". Below this, there are five main categories of web apps, each with a representative image and a label:

- Optimization for SOL 200**: Shows a 3D model of a mechanical part in two states, "Before" and "After", illustrating topology optimization.
- Multi Model Optimization**: Shows a 3D model of a mechanical part with arrows indicating a process flow or optimization path.
- Machine Learning | Parameter Study**: Shows four small plots representing different machine learning or parameter study results.
- HDF5 Explorer**: Shows a line graph with multiple data series, representing the extraction of results from an HDF5 file.
- Remote Execution**: Shows a diagram of data flow between a "Remote System" and a "Local System", with "Input Files" being sent to the remote system and "Results Files" being received back.

At the bottom of the interface, there are two additional links: "Tutorials and User's Guide" and "Full list of web apps". A red circle with the number "1" is placed over the "Machine Learning | Parameter Study" category, indicating the link to click.



Select BDF Files

1

1. Select files

nas103_ws07_with_spring_support.dat

Inspecting: 100%

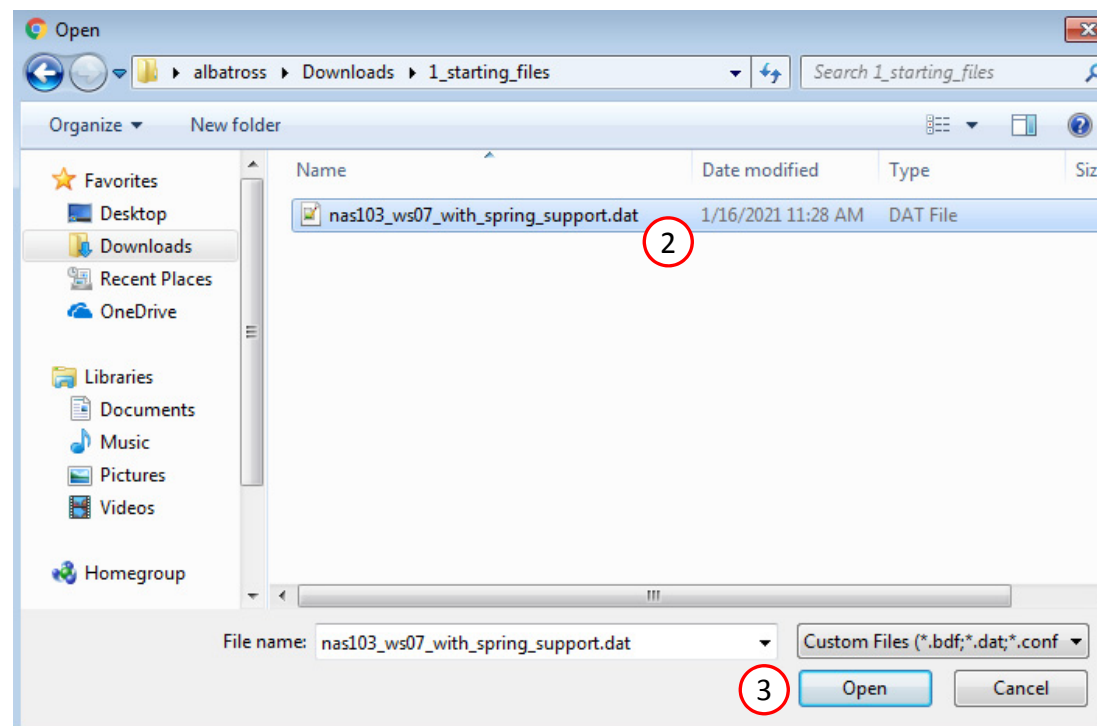
4

2. Upload files

Uploading: 100 %

Select BDF Files

1. Click Select files
2. Select the indicated files
3. Click Open
4. Click Upload files



Parameters

- Set the following fields as parameters
 - x1: The spring stiffness of PELAS 20
- Parameters have been created for the selected fields
- For each parameter, use the following settings:
 - Low: .1
 - High: 10.

- Bulk data entries will always be displayed in the small field format.
- Only fields that have real or integer data entries may be selected as parameters. If the field is blank or contains only characters, the field may not be selected.

Select Parameters

\$ _1_ _2_ _3_ _4_ _5_ _6_ _7_						
EIGB	30	INV	0.	3.	20	2
FORCE	6	2		1.	0.	-1. 0.
MAT1	1	10.E7				
PELAS	20	%x1%				
PROD	10	1	.1			

Configure Parameters

Delete	Parameter	Status	Low	High	Comments
(2) ✖	x1	✔	.1	10.	Field 3 of P

Responses

1. Click Responses
2. Click Select files
3. Select the indicated file
4. Click Open
5. Click Upload files

1

Upload .h5 File

2

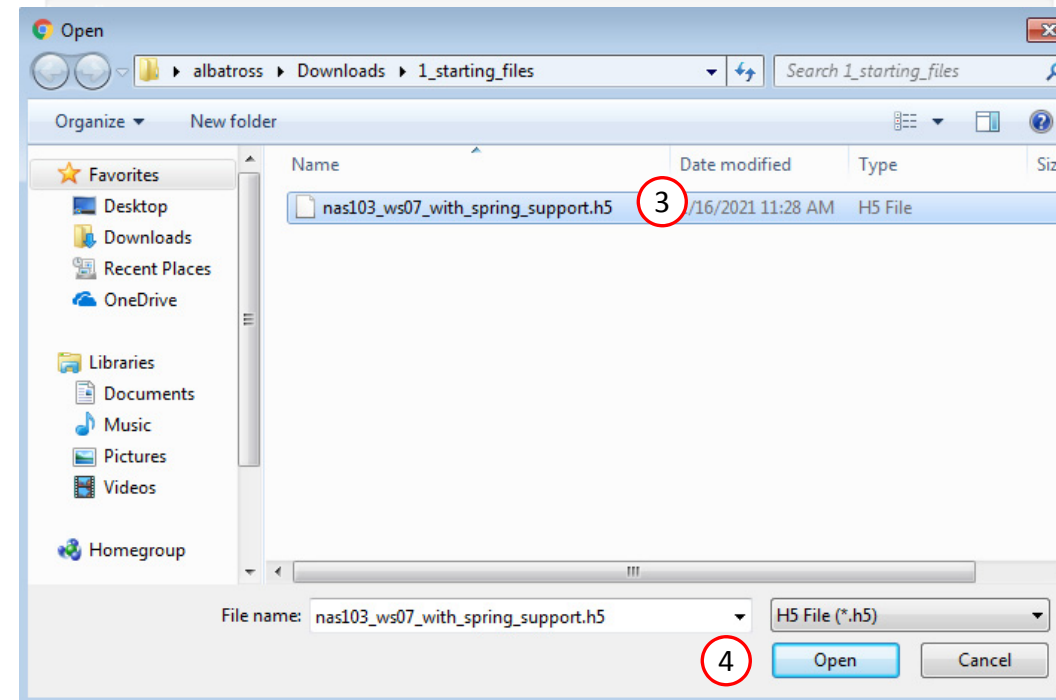
1. Select files

nas103_ws07_with_spring_support.h5

5

2. Upload files

Uploading



Adjust the Column Width

1. Optional - Use at your liking the buttons at the top right hand corner to adjust the width of the left and right columns

SOL 200 Web App - Machine Learning

Parameters Samples Responses Download Results

Connection Settings Home

Select Responses to Monitor

Session ID: 3710

HDF5

Select Dataset

- NODAL/ACCELERATION
- NODAL/DISPLACEMENT
- NODAL/GRID_WEIGHT
- NODAL/VELOCITY_CPL
- SUMMARY/EIGENVALUE

Acquired Dataset

NODAL/GRID_WEIGHT - 0

Reset Filters

SAMPLE	DOMAIN_ID	SUBCASE	STEP	ANA

View Responses to Monitor

Monitored Responses

Hide/Show Columns Reset Filters

Download CSV

Delete	Label	Status	Objective	Lower Bound	Upper Bound	Monitor the Fil cycle (SO)
	r1			Lower	Upper	

Select Responses to Monitor

Session ID: 3710 HDF5

Select Dataset

- NODAL/ACCELERATION_CPLX
- NODAL/DISPLACEMENT_CPLX
- NODAL/GRID_WEIGHT**
- NODAL/VELOCITY_CPLX
- SUMMARY/EIGENVALUE

Specify Entities

(ID)

Examples: 0, etc.

Acquired Dataset Reset Filters

NODAL/GRID_WEIGHT - 0

SAMPLE	DOMAIN_ID	SUBCASE	STEP	ANALYSIS	TIME_FREQ_EIGR	
name of H5 File**		Subcase number	Step number	Analysis type	Time, frequency or real part of eigen value	Im eig apl
model		0	0	0	0	

View Responses to Monitor

Monitored Responses Hide/Show Columns Reset Filters Download CSV

Delete	Label	Status	Objective	
✖	r1	✔	<input type="text"/>	Lc

5 10 20 30 50 100

Select Responses

1. Select the following dataset:
SUMMARY/EIGENVALUE
2. Use the horizontal scroll bar until the column TIME_FREQ_EIGR is visible
3. A new response r1 is created

SOL 200 Web App - Machine Learning Parameters Samples Responses Download Results Connection Settings Home

Session ID: 9465 HDF5

Select Responses to Monitor

Select Dataset

- ELEMENTAL/ELEMENT_F
- ELEMENTAL/ELEMENT_F
- NODAL/DISPLACEMENT
- NODAL/EIGENVECTOR
- SUMMARY/EIGENVALUE**

Specify Entities

1

(MODE)

Examples: 1, etc..

☒ Auto Execute

Acquire Dataset

✓ Acquisition complete and successful

Acquired Dataset

SUMMARY/EIGENVALUE - 1

MODE	ORDER	EIGEN	OMEGA
1	1	10.0015003...	3.16251487...

1

2

View Responses to Monitor

Monitored Responses

Hide/Show Columns Reset Filters Download CSV

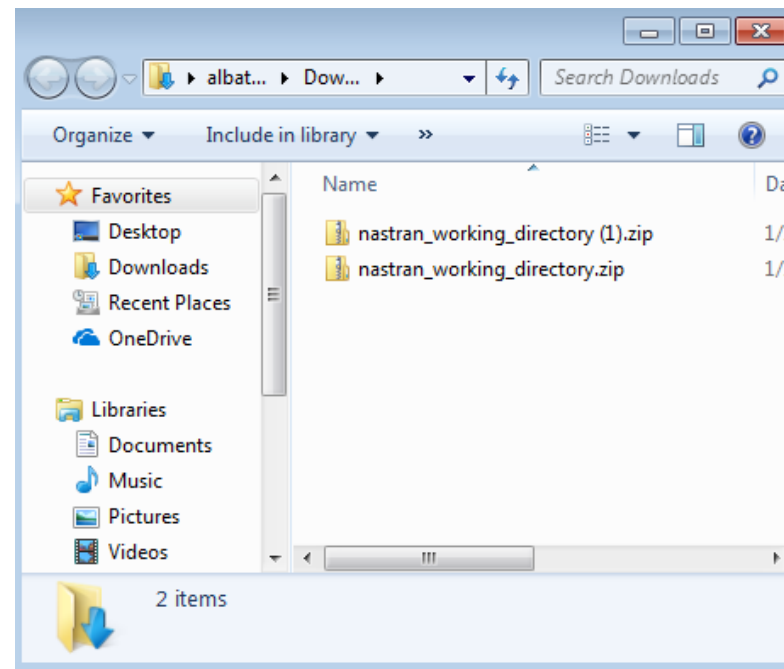
Delete	Label	Status	Objective	Lower Bound	Upper Bound	Monitor the re of the FINAL cycle (SOL 20
3	r1	+	▼	Lower	Upper	

5 10 20 30 50 100

Configuring Multiple Batch Runs

Samples

In the following slides, we will configure 2 batches to run.



Batch	File Name	Number of Runs	Purpose
1	nastran_working_directory.zip	10	The data from these 10 runs is used to train the surrogate model.
2	nastran_working_directory (1).zip	20	The data from these 20 runs is compared with the predictions from the surrogate model. The normalized root mean square error (NRMSE) is calculated based on these 20 runs.

Samples

1. Click Samples
2. Ensure the following design is selected:
Latin Hypercube, Reproducible
3. Set Number of Samples to 10
4. The samples have been updated, note that
samples 1, 2, 3, ..., 10 are visible
5. The indicated controls can be used to
display the other samples

SOL 200 Web App - Machine Learning Parameters **Samples** Responses Download Results Connection Settings Home

1

Configure Samples

Design

Latin Hypercube, Reproducible 2

+ Info

Number of Samples

10 3

→

Samples to Run

+ Options

4

Sample Number	Parameters
1	x1 1.208613
2	5.371329
3	9.449995
4	4.353574
5	6.326213

5

« 1 2 » 5 10 20 30 40 50

◀ ▶

Download

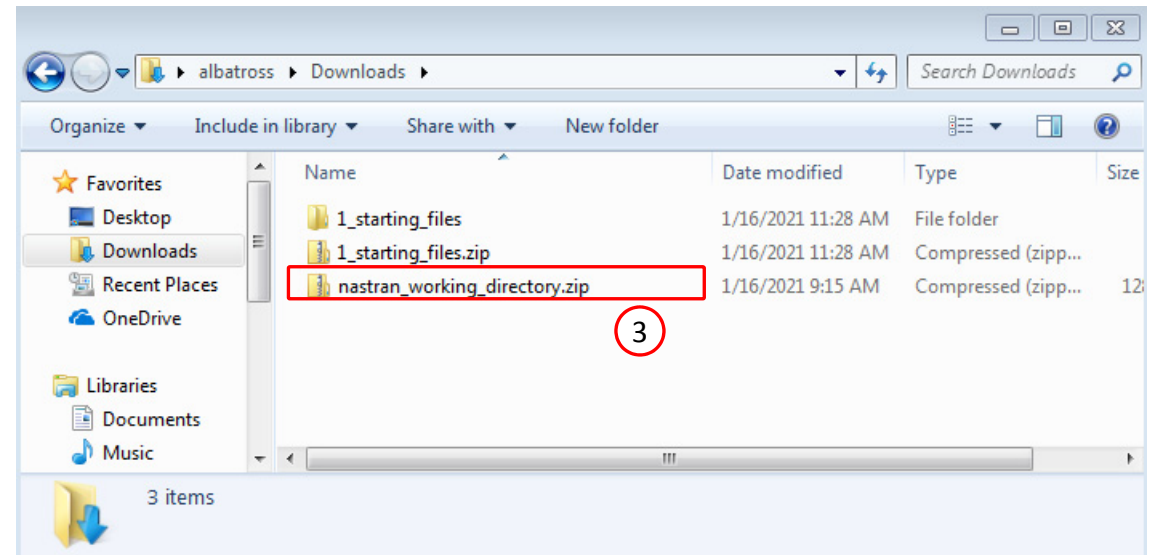
1. Click Download
2. Click Download BDF Files
3. A new ZIP file has been downloaded

1

Download

Download BDF Files

2



Samples

1. Click Samples
2. Ensure the following design is selected:
Latin Hypercube, Reproducible
3. Set Number of Samples to 20
4. The samples have been updated, note that
samples 1, 2, 3, ..., 20 are visible
5. The indicated controls can be used to
display the other samples

SOL 200 Web App - Machine Learning Parameters **Samples** Responses Download Results Connection Settings Home

◀ ▶

Configure Samples

Design

Latin Hypercube, Reproducible

+ Info

Number of Samples

20

→

Samples to Run

+ Options

Sample Number	Parameters
1	8.740013
2	6.337985
3	9.193342
4	4.064234
5	1.611121

« 1 2 3 4 » 5 10 20 30 40 50

◀ ▶

Download

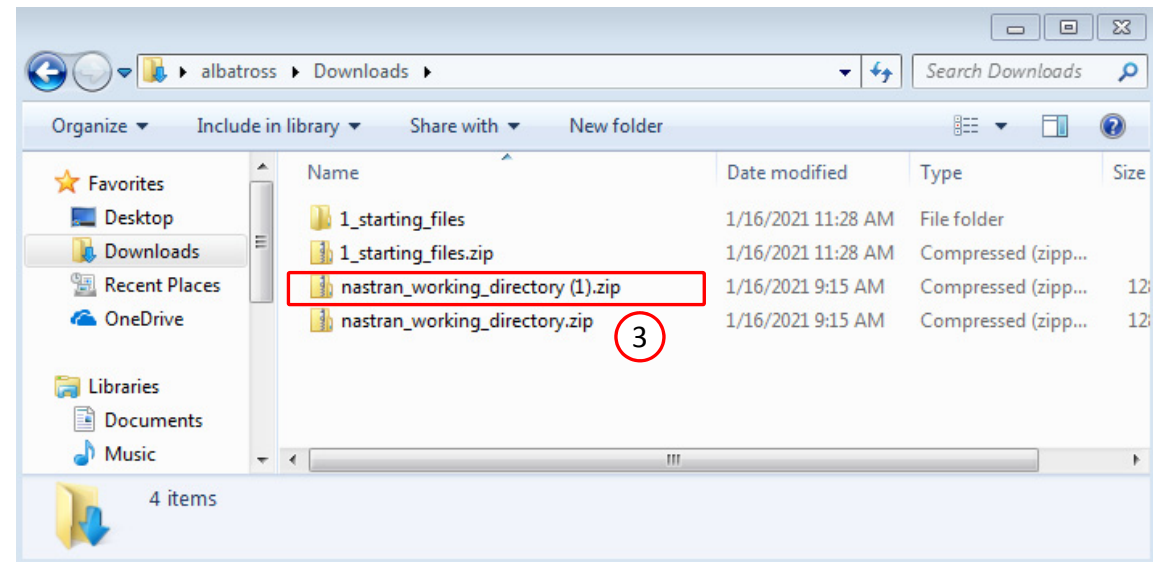
1. Click Download
2. Click Download BDF Files
3. A new ZIP file has been downloaded

1

Download

Download BDF Files

2



Parameters

1. Click Parameters
2. For each parameter, use the following settings:
 - Low: 1.0
 - High: 40.0

SOL 200 Web App - Machine Learning

Parameters Samples Responses Download Results Connection Settings Home

1

Select Parameters

Configure Parameters

Delete	Parameter	Status	Low	High	Comments
	x1		1.0	40.0	Field 3 of P

2

\$ _1 _ || _2 _ || _3 _ || _4 _ || _5 _ || _6 _ || _7 _ || _8 _ || _9 _ || _10 _ |

EIGB	30	INV	0.	3.	20	2	2
FORCE	6	2		1.	0.	-1.	0.
MAT1	1	10.E7					
PELAS	20	%x1%					
PROD	10	1	.1				

Samples

1. Click Samples
2. Set the Design as Mesh Grid
3. Set the Number of Samples as 40
4. The table now has 40 samples
5. Click +Options
6. Click Export
7. A CSV file has been download and contains the values from the table with 8 samples

- Later in the tutorial, the 40 sample points in the CSV file will be used to make predictions.

SOL 200 Web App - Machine Learning Parameters **Samples** Responses Download Results Connection Settings Home

◀ ▶

Configure Samples

Design

Mesh Grid **2**

[+ Info](#)

Number of Design Points Per Parameter

40 **3**

This configuration will generate a design with 40 runs

Samples to Run

[+ Options](#) **5**

CSV Export

[Export](#) **6**

4

Sample Number	Parameters
	x1
1	1.
2	2.
3	3.
4	4.
5	5.

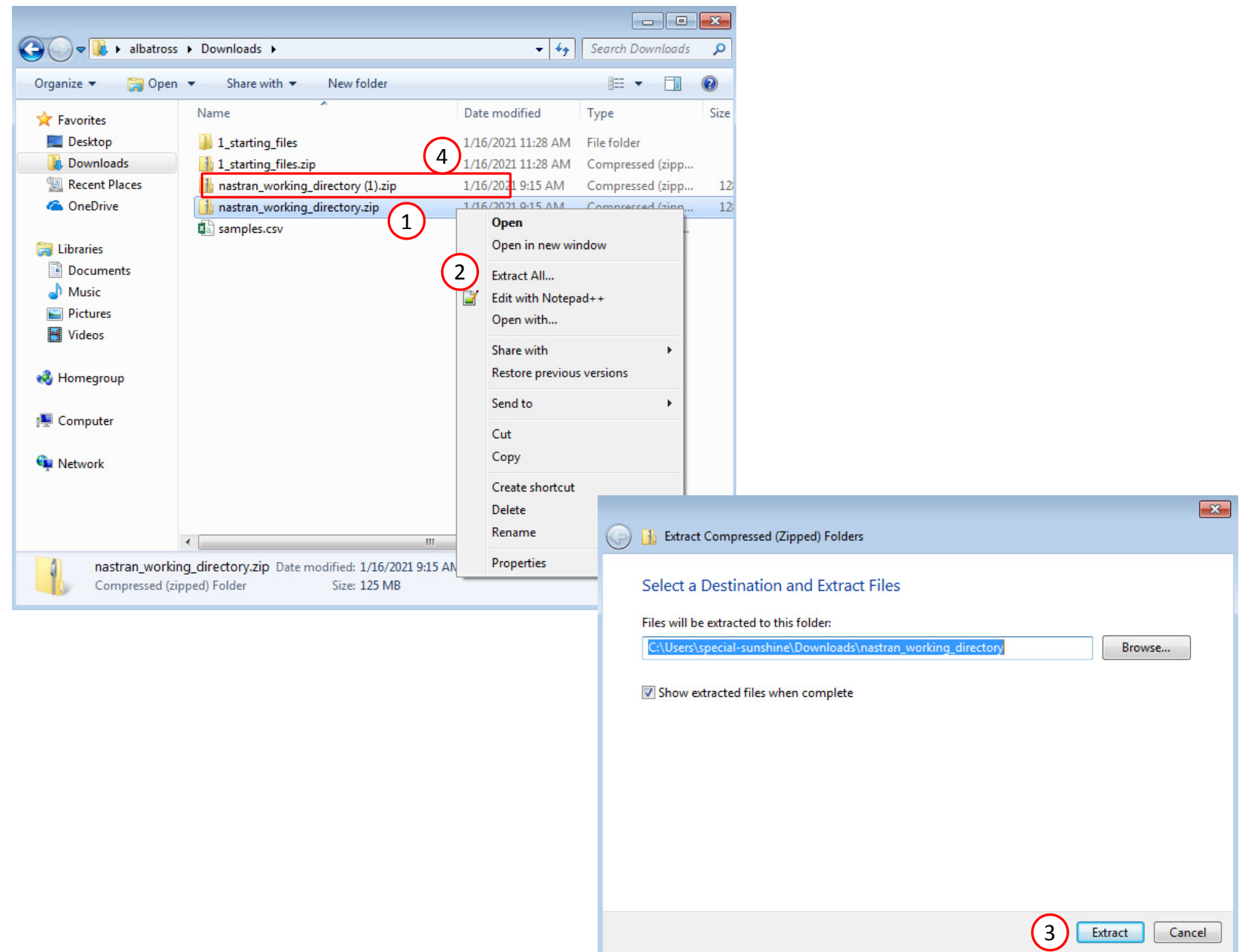
5 10 20 30 40 50

« 1 2 3 4 5 6 7 8 »

Start Desktop App

1. Right click on the indicated file
2. Click Extract All
3. Click Extract on the following window
4. Repeat steps 1-3 for the indicated files

- Always extract the contents of the ZIP file to a new, empty folder.



Start Desktop App

1. Open this folder:
nastran_working_directory
2. Inside of the new folder, double click on
Start Desktop App
3. Click Open, Run or Allow Access on any
subsequent windows
4. MSC Nastran will now start

- One can run the Nastran job on a remote machine as follows:
1) Copy the BDF files and the INCLUDE files to a remote machine. 2) Run the MSC Nastran job on the remote machine. 3) After completion, copy the BDF, F06, LOG, H5 files to the local machine. 4) Click "Start Desktop App" to display the results.

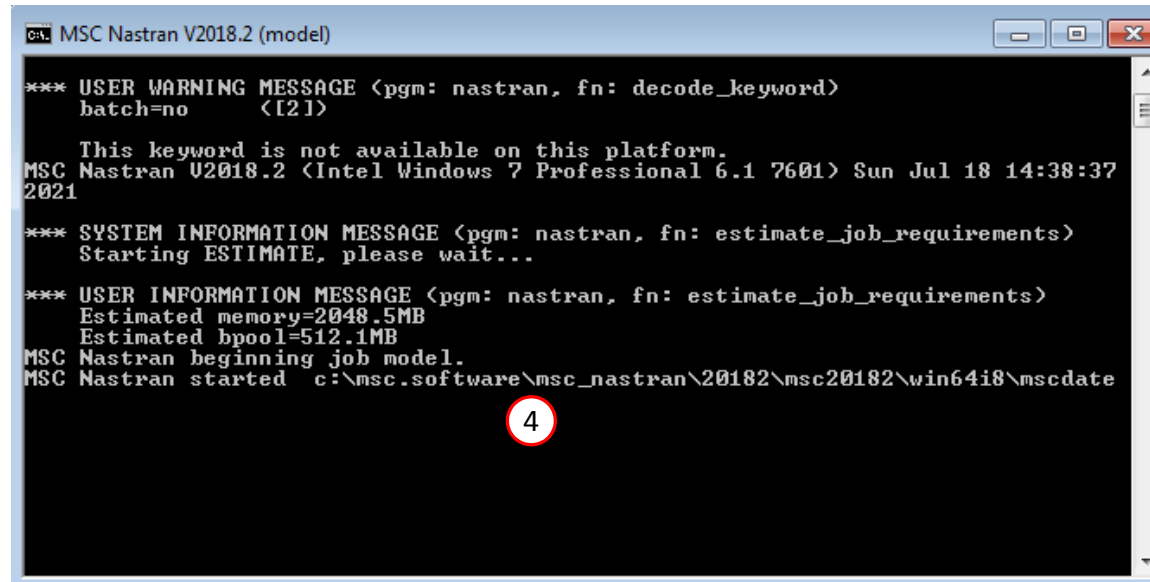
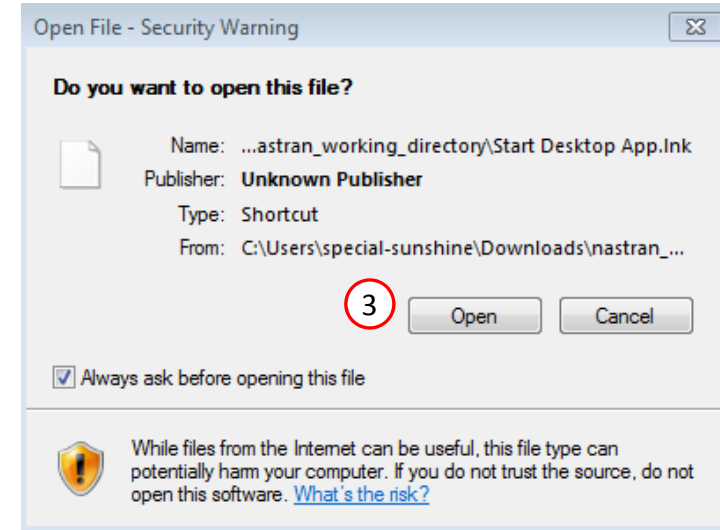
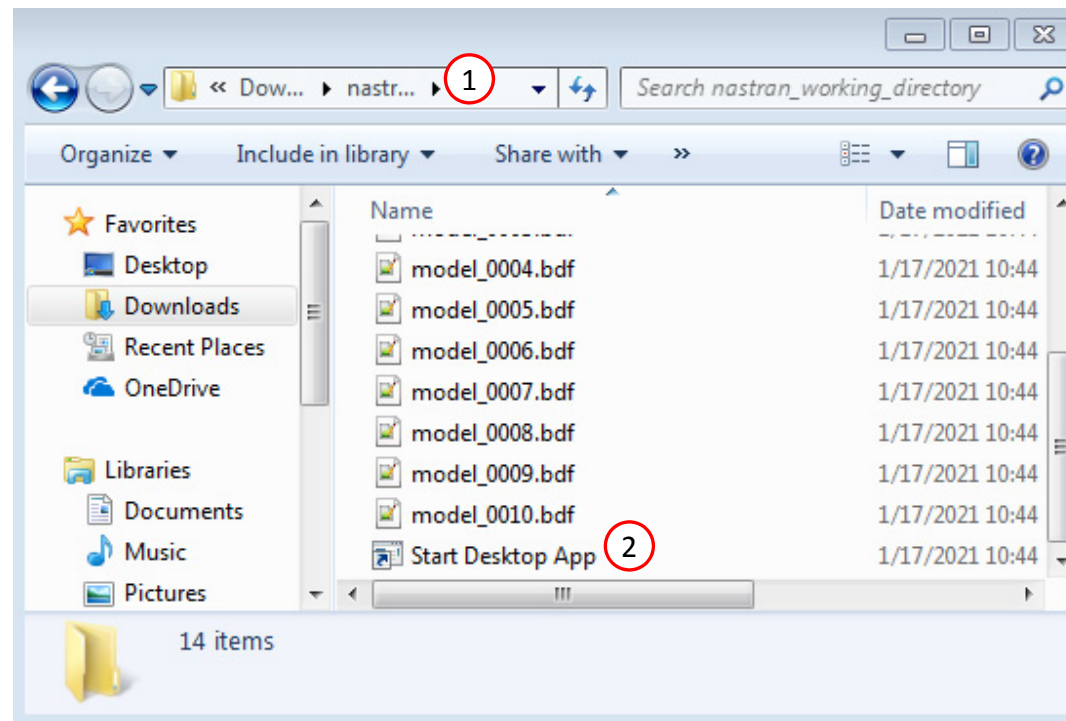
Using Linux?

Follow these instructions:

- 1) Open Terminal
- 2) Navigate to the nastran_working_directory
`cd ./nastran_working_directory`
- 3) Use this command to start the process
`./Start_MSC_Nastran.sh`

In some instances, execute permission must be granted to the directory. Use this command. This command assumes you are one folder level up.

```
sudo chmod -R u+x ./nastran_working_directory
```




Status

- While MSC Nastran is running, a status page will show the current state of MSC Nastran

SOL 200 Web App - Status

 Python

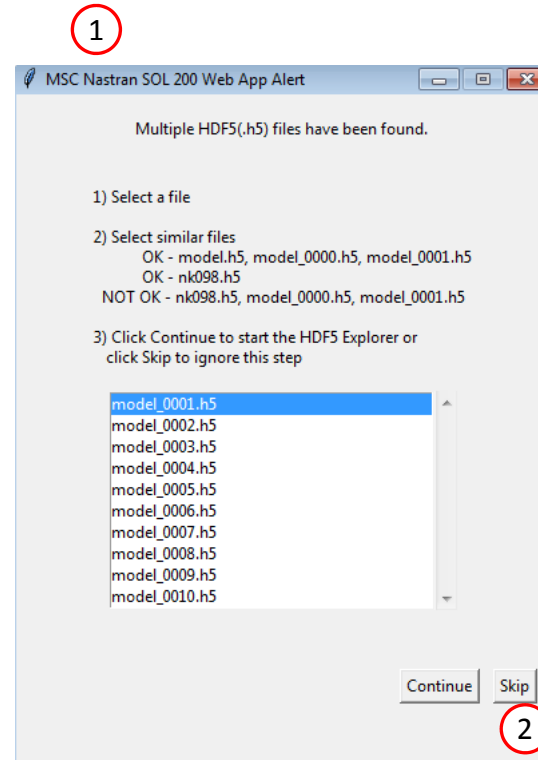
 MSC Nastran

Status

Name	Status of Job	Design Cycle	RUN TERMINATED DUE TO
model.bdf	Running	None	

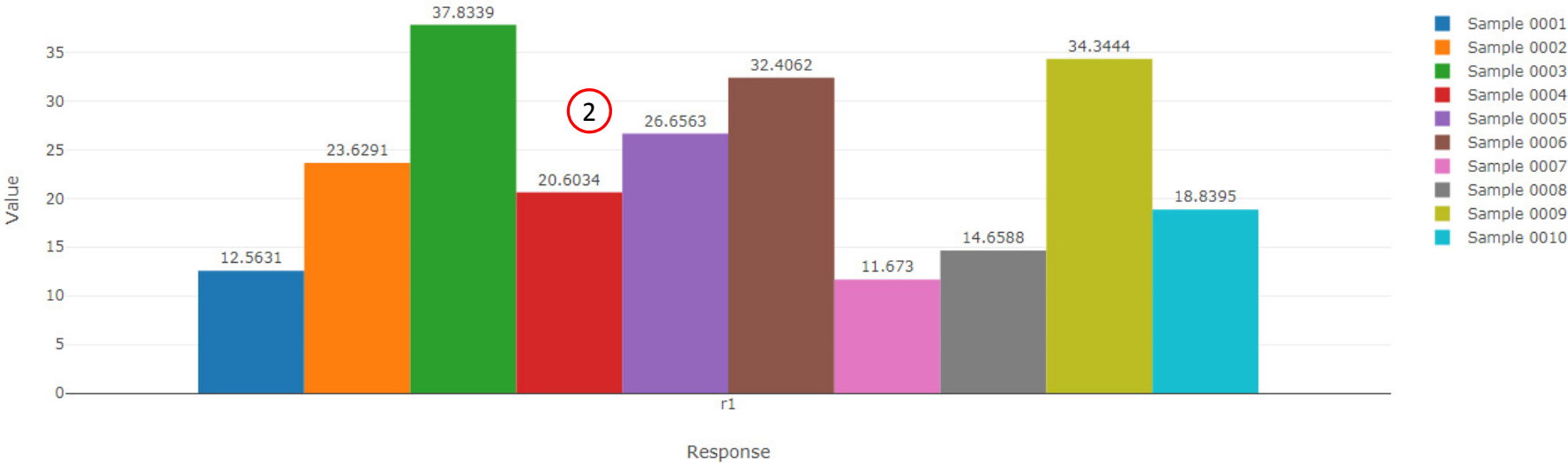
Review Results

1. A window appears asking to start the HDF5 Explorer
2. Click Skip to not open the HDF5 Explorer



Review Results

- 1. The Monitored Responses web app is opened
- 2. The value of each response and for each sample is displayed in a bar chart
- 3. A table lists the values for each response and sample.



B

Monitored Responses

Display MAX and MIN Download CSV Reset Filters

Label	Dataset Name	Field	Field Description	Current Value
r1	SUMMARY/EIGENVALUE	EIGEN		
r1	SUMMARY/EIGENVALUE	EIGEN		10.001500337521877

3

Monitored Responses from Each Sample

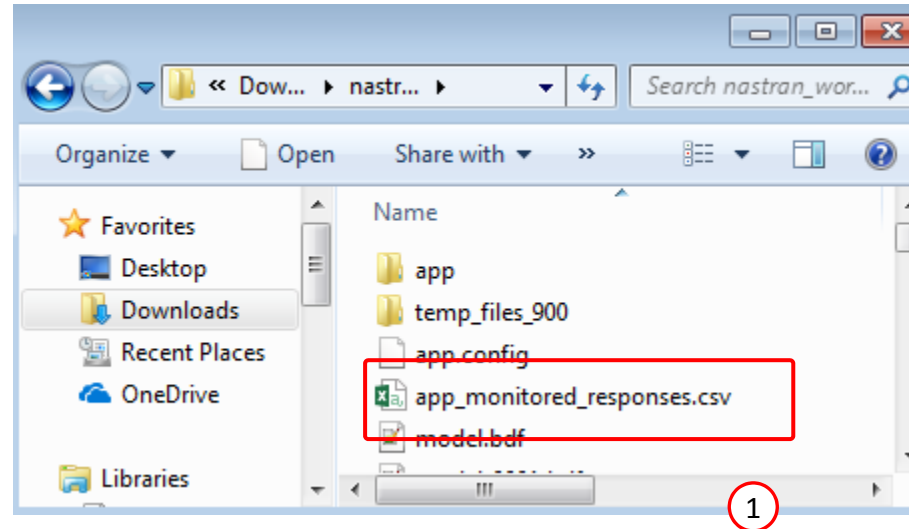
0001	0002	0003	0004	
12.563078819847316	23.62907115939849	37.8338533140817	20.60335328534742	26.6

- A. The table titled Monitored Response can be interacted with. Each column in the table contains filters. Once a filter is modified, the Bar Chart will instantly update.
- B. Additional functions include the ability to highlight the MAX and MIN bars, download a CSV file and reset the filters.

Review Results

1. The monitored responses are contained in the CSV file named `app_monitored_responses.csv`

The responses in this CSV file will be used to train the surrogate model.

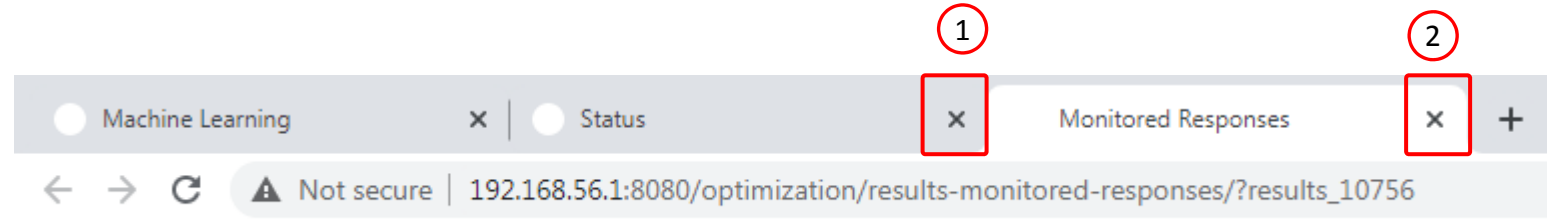


A screenshot of an Excel spreadsheet titled 'app_monitored_responses.csv - Excel'. The spreadsheet shows a table with columns A through J. Column A is labeled 'Sample' and contains values 1 through 6. Columns B through J contain numerical data. The table is highlighted with a red border.

	A	B	C	D	E	F	G	H	I	J
1	Sample	r1	r2	r3	r4	r5	r6	r7	r8	r9
2	1	1217.217	7053.424	25842.42	5181.517	7655.089	111.5268	121.4934	105.4131	117.6776
3	2	1505.006	8540.09	25683.63	4366.002	9054.831	114.3995	121.8412	111.7995	119.8613
4	3	1138.427	6955.114	26141.29	3893.004	8777.485	113.8775	122.2895	107.8186	120.776
5	4	1014.942	6958.814	23340.53	4311.815	6015.679	109.3869	116.1823	108.7163	114.8376
6	5	1379.038	8133.175	28819.79	4774.838	8635.851	113.6273	120.3388	108.8235	117.9242

Close Pages

1. The Status page can be closed
2. The Monitored Responses page can be closed



Start Desktop App

1. Open this folder:
nastran_working_directory (1)
2. Inside of the new folder, double click on
Start Desktop App
3. Click Open, Run or Allow Access on any
subsequent windows
4. MSC Nastran will now start

- One can run the Nastran job on a remote machine as follows:
1) Copy the BDF files and the INCLUDE files to a remote machine. 2) Run the MSC Nastran job on the remote machine. 3) After completion, copy the BDF, F06, LOG, H5 files to the local machine. 4) Click "Start Desktop App" to display the results.

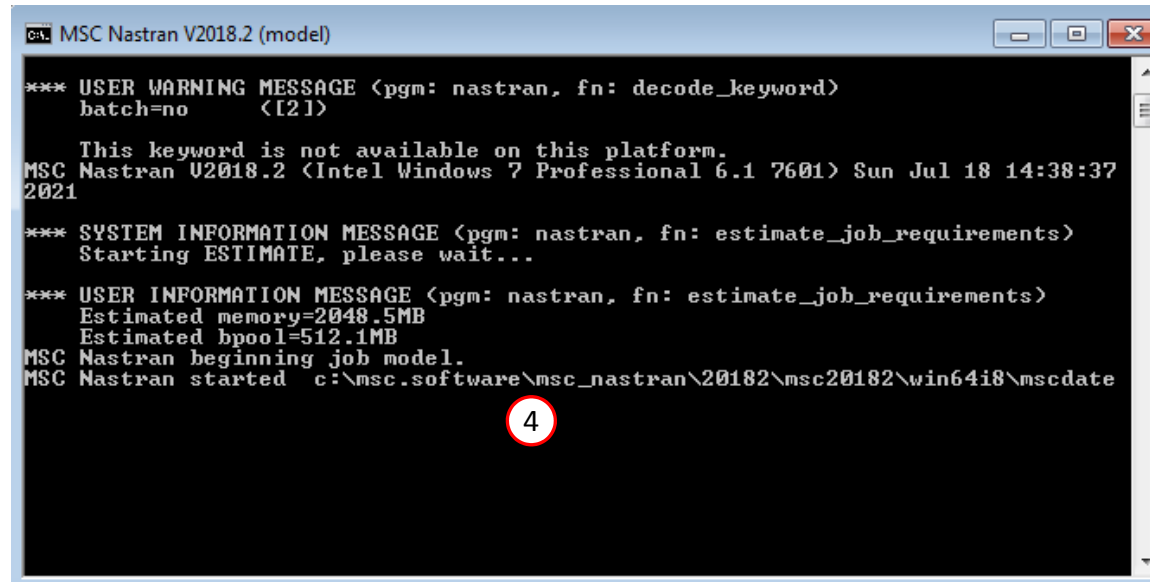
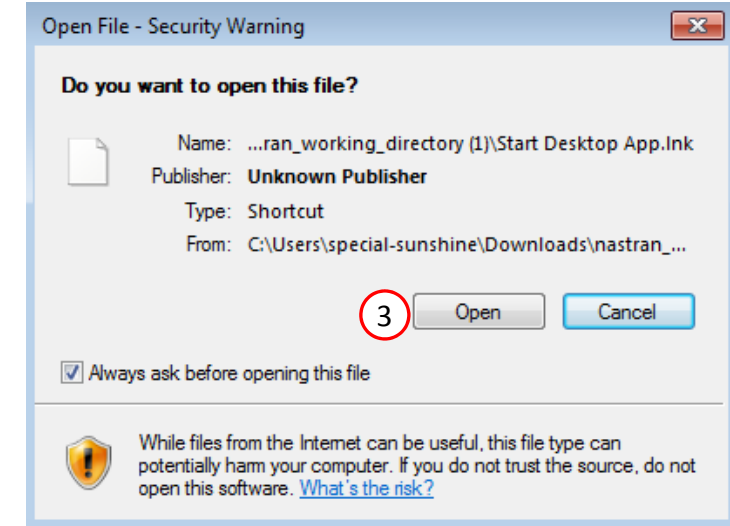
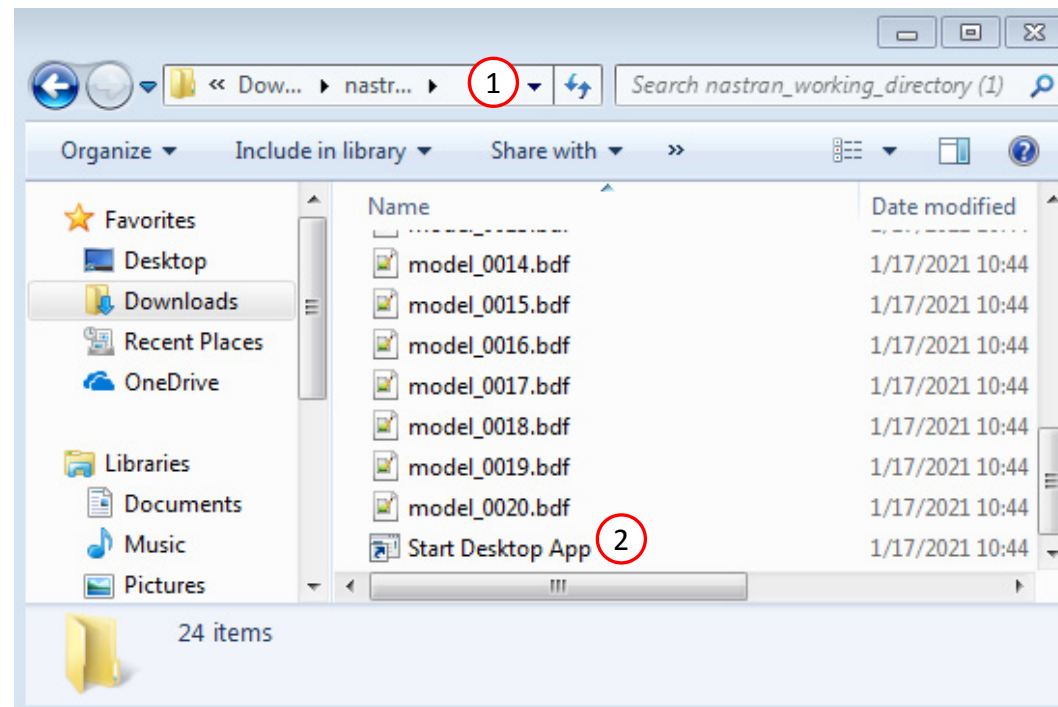
Using Linux?

Follow these instructions:

- 1) Open Terminal
- 2) Navigate to the nastran_working_directory
`cd ./nastran_working_directory`
- 3) Use this command to start the process
`./Start_MSC_Nastran.sh`

In some instances, execute permission must be granted to the directory. Use this command. This command assumes you are one folder level up.

```
sudo chmod -R u+x ./nastran_working_directory
```



Status

- While MSC Nastran is running, a status page will show the current state of MSC Nastran

SOL 200 Web App - Status

 Python

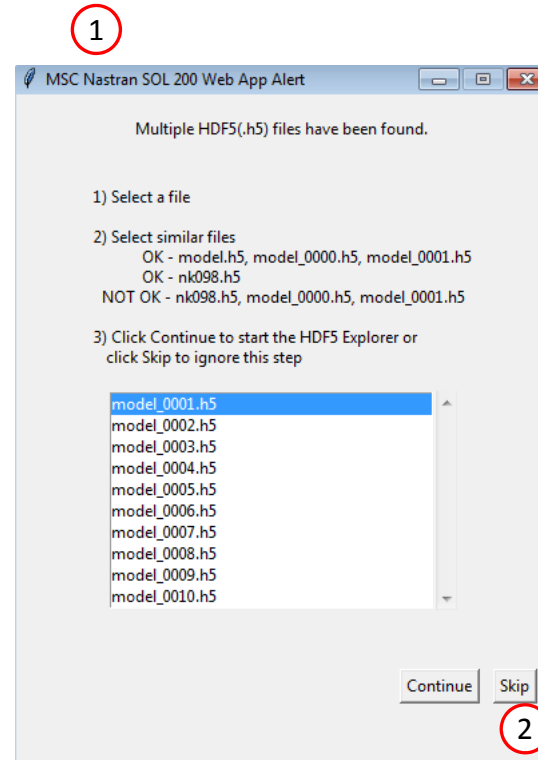
 MSC Nastran

Status

Name	Status of Job	Design Cycle	RUN TERMINATED DUE TO
model.bdf	Running	None	

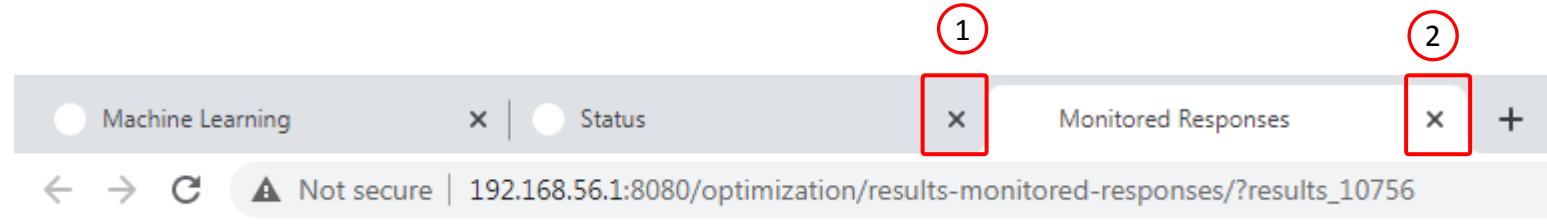
Review Results

1. A window appears asking to start the HDF5 Explorer
2. Click Skip to not open the HDF5 Explorer



Close Pages

1. The Status page can be closed
2. The Monitored Responses page can be closed



Performing Predictions

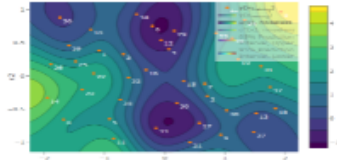
Prediction Analysis Web App

1. Return to the Machine Learning web app
2. Click Results
3. Click Prediction Analysis
4. The Prediction Analysis web app is now open
5. Ensure it says Connected

SOL 200 Web App - Machine Learning Parameters Samples Responses Download **Results** Connection Settings Home

1 2

Select a Results App

 3

Prediction Analysis

SOL 200 Web App - Prediction Analysis 4 Home

Gaussian Process (GP) App Connection Status

✓ Connected 5

Session ID: 8207

Output

```
GP App Update - Starting the Gaussian Process (GP) app on the server
- Session ID: 8207
- Address: http://localhost:8080/optimization
Desktop App Update - Connecting to the SOL 200 Web App...
GP App Update - Connection successful between the Node JS server and GP ap
```

Warnings and Errors

Warnings can be ignored

Training Data

1. Navigate to the Training and Testing Data section
2. Delete any previous table data by clicking the four (4) buttons named Delete all rows

- **x_training, y_training** - This specifies the x inputs and y outputs used to train the surrogate model.
- **x_testing, y_testing** - This specifies the x inputs and y outputs used to calculate the Normalized Root Mean Square Error (NRMSE) between the predicted values and actual MSC Nastran responses. This testing data is optional.
- **x_prediction** – The x inputs at which to make predictions.

Training and Testing Data 1

x_training

CSV Export



CSV Import



Select a CSV File



CSV

imported

y_training

CSV Export



CSV Import



Select a CSV File



x_testing

CSV Export



CSV Import



Select a CSV File



y_testing

CSV Export



CSV Import



Select a CSV File

2

✕ Delete all rows

✕ Delete all rows

✕ Delete all rows

✕ Delete all rows

Training Data

1. Navigate to the section titled x_training
2. Click Select files
3. Navigate to the folder named nastran_working_directory which contains data for 10 runs
4. Select the file app.config
5. Click Open
6. Click Import
7. The table is now loaded with the x inputs for all 10 runs

x_training **1**

CSV Export CSV Import **6**

2 Export Select files app.config Import **6** CSV imported

7

Delete all rows

sample	x1
1	1.208613
2	5.371329
3	9.449995
4	4.353574
5	6.326213
6	8.000973
7	.8043
8	2.107346
9	8.531418
10	3.725496

10 25 50 100

Open

File name: app.config

Custom Files (*.csv;*.config)

Open Cancel

Training Data

1. Navigate to the section titled y_training
2. Click Select files
3. Navigate to the folder named nastran_working_directory which contains data for 10 runs
4. Select the file app_monitored_responses.csv
5. Click Open
6. Click Import
7. The table is now loaded with the y outputs (monitored responses) for all 10 runs

y_training 1

CSV Export CSV Import 6

Export Select files app_monitored_responses.csv Import 2

CSV imported

7

Delete all rows

sample	y1
0001	12.563078819...
0002	23.6290711593...
0003	37.833853314...
0004	20.603353285...
0005	26.656288971...
0006	32.406203636...
0007	11.6729669201...
0008	14.658815254...
0009	34.344371393...
0010	18.839516190...

10 25 50 100

Open

Downloads nastran_working_directory 3

Search nastran_working_direct...

Organize New folder

Name	Date modified	Type	Size
app	1/16/2021 9:16 AM	File folder	
temp_files_900	1/16/2021 12:06 PM	File folder	
app.config	1/16/2021 9:16 AM	CONFIG File	
app_monitored_responses.csv	1/16/2021 9:22 AM	Microsoft Excel C...	

4

File name: app_monitored_responses.csv 5

Custom Files (*.csv;*.config)

Open Cancel

Testing Data

1. Navigate to the section titled x_testing
2. Click Select files
3. Navigate to the folder named nastran_working_directory (1) which contains data for 20 runs
4. Select the file app.config
5. Click Open
6. Click Import
7. The table is now loaded with the x inputs for all 20 runs

x_testing 1

CSV Export CSV Import 6

Export Select files app.config Import 2

CSV imported

7

Delete all rows

sample	x1
1	8.740013
2	6.337985
3	9.193342
4	4.064234
5	1.611121
6	3.980258
7	6.734346
8	5.203433
9	.9947
10	2.740009

« 1 2 » 10 25 50 100

Open

« Downloads » nastran_working_directory (1) 3 Search nastran_working_direct...

Organize New folder

File name: app.config 5 Custom Files (*.csv;*.config) Open Cancel

4

app temp_files_900 app.config app_monitored_responses.csv

1/16/2021 9:16 AM 1/16/2021 9:21 AM 1/16/2021 9:16 AM 1/16/2021 9:20 AM

File folder File folder CONFIG File Microsoft Excel C...

Testing Data

1. Navigate to the section titled y_testing
2. Click Select files
3. Navigate to the folder named nastran_working_directory (1) which contains data for 20 runs
4. Select the file app_monitored_responses.csv
5. Click Open
6. Click Import
7. The table is now loaded with the y outputs (monitored responses) for all 20 runs

y_testing 1

CSV Export CSV Import 6

Export Select files app_monitored_responses.csv Import 2

CSV imported

7

sample	y1
0001	35.121966603...
0002	26.694747347...
0003	36.841889515...
0004	19.780993665...
0005	13.481700246...
0006	19.545453554...
0007	28.005814381...
0008	23.1156551662...
0009	12.088066524...
0010	16.231018676...

« 1 2 » 10 25 50 100

Open

« Downloads » nastran_working_directory (1) 3 Search nastran_working_direct...

Organize New folder

Name	Date modified	Type	Size
app	1/16/2021 9:16 AM	File folder	
temp_files_900	1/16/2021 9:21 AM	File folder	
app.config	1/16/2021 9:16 AM	CONFIG File	
app_monitored_responses.csv	1/16/2021 9:20 AM	Microsoft Excel C...	

4


File name: app_monitored_responses.csv Custom Files (*.csv;*.config) 5 Open Cancel

Perform Regression

1. Click Perform Regression and the surrogate model will be fitted
2. The regression is complete when the following status message is visible:
 - Process complete

Regression

Data	Link to Table	Status	Status Description
x_training	Link	✓	Ready
y_training	Link	✓	Ready
x_testing (Optional)	Link	✓	Ready
y_testing (Optional)	Link	✓	Ready

 Perform Regression

1

✓ Process complete

2

[Click here](#) to view the Regression Results section

Output

```
| Response | x1 |
|:-----|:-----:|
| y1       | 39.434 |

Parameters listed in decreasing order of relevance: x1
GP App Update - Sending initial data to the web browser
GP App Update - Sending complete
```

Warnings and Errors

```
/home/apricot/PycharmProjects/python-app/venv/lib/python3.6/site-packages/GPy/ke
/home/apricot/PycharmProjects/python-app/venv/lib/python3.6/site-packages/GPy/ke
/home/apricot/PycharmProjects/python-app/venv/lib/python3.6/site-packages/GPy/ke
/home/apricot/PycharmProjects/python-app/venv/lib/python3.6/site-packages/GPy/ke
```

Warnings can be ignored

Perform Prediction

1. Navigate to the section titled x_prediction
2. Click Select files
3. Navigate to the location of the file named samples.csv
4. Select the file samples.csv
5. Click Open
6. Click Import
7. The table is now loaded with the x inputs for 40 runs

Prediction

x_prediction 1

CSV Export



CSV Import



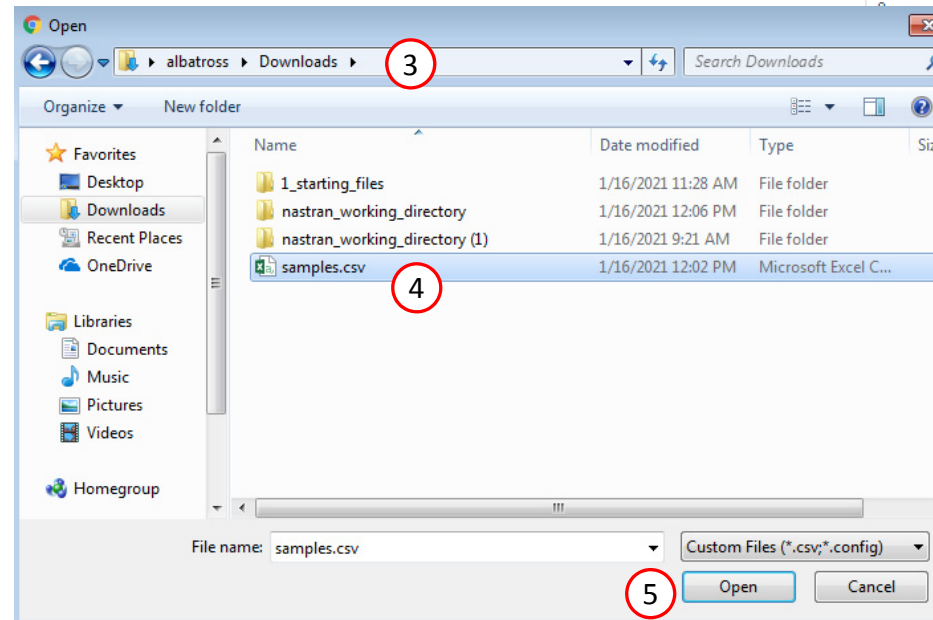
samples.csv



✓ CSV
imported

✕ Delete all rows

sample	x1
1	1.
2	2.
3	3.
4	4.
5	5.
6	6.
7	7.
8	8.
9	9.
10	10.




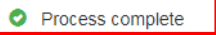
Perform Prediction

1. Navigate to the section titled Perform Prediction
2. Click Perform Prediction
3. The prediction is complete when the following status message is visible:
 - Process complete

- Note that the predictions are performed seemingly instantly

Perform Prediction ¹

 ²

 ³

[Click here](#) to view the Prediction Results section

Output

```
GP App Update - The web browser has requested a prediction
GP App Update - Determining prediction
GP App Update - Normalizing Design - Scaling and shifting the input space to [0,1]
GP App Update - Sending prediction data to the web browser
GP App Update - Sending complete
```

Warnings and Errors

Warnings can be ignored

Variance

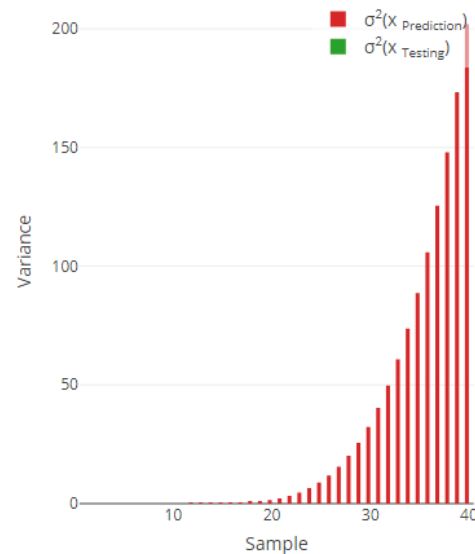
1. Navigate to the section titled Variance
2. Note the normalized root mean square error (NRMSE)
 - NRMSE values are only calculated if `x_testing` and `y_testing` are provided
 - NRMSE values less than .15 indicate the surrogate model has good prediction performance

- **x_training, y_training** - This specifies the x inputs and y outputs used to train the surrogate model.
- **x_testing, y_testing** - This specifies the x inputs and y outputs used to calculate the Normalized Root Mean Square Error (NRMSE) between the predicted values and actual MSC Nastran responses. This testing data is option.
- **x_prediction** – The x inputs at which to make predictions.

Variance 1

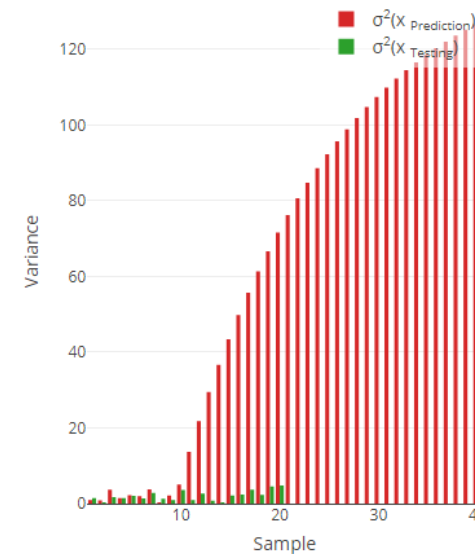
Matern52 2

NRMSE: 8.863379504119915e-06



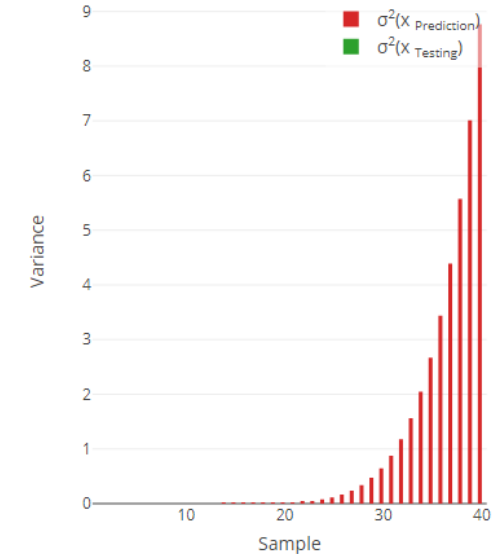
Exponential

NRMSE: 0.019861846267229557



RBF

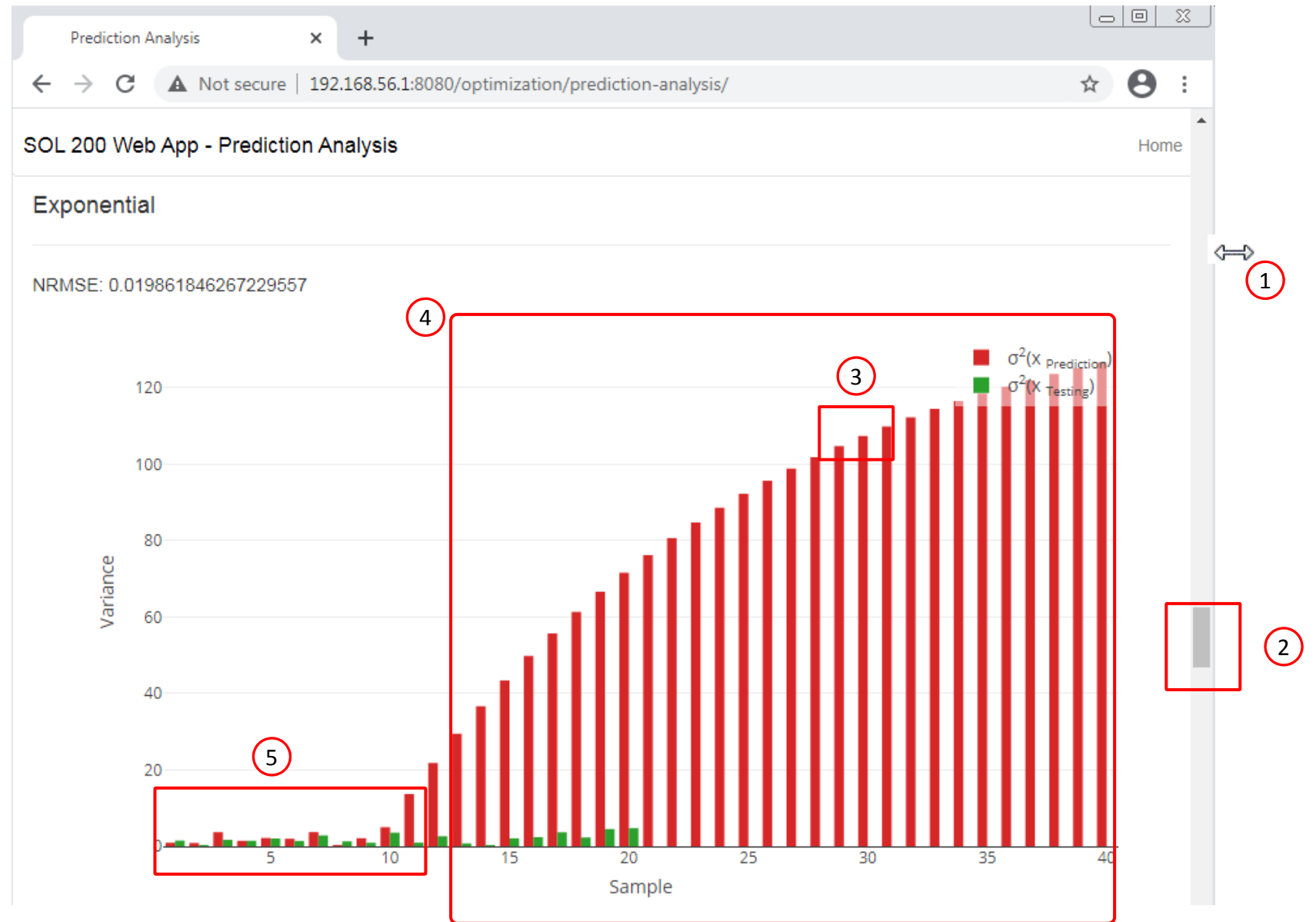
NRMSE: 1.2399877479780946e-05



Variance

1. Resize the window to fit half the screen, this causes the plot to be increased in size
2. Adjust the scroll bar to make the plot visible
3. A high bar indicates a high prediction uncertainty, or a high variance, and is indication that we do not have enough information to conclude the prediction is credible at that prediction point.
4. Note the variance (prediction uncertainty) is high for many of the prediction points (red bars). The x inputs of the original training data was within the bounds of .01 and 10.0, so the surrogate model is valid within these bounds. The prediction points are within the bounds of 1.0 and 40.0 Predictions made outside of these bounds result in high variance (high prediction uncertainty).
5. The first 10 samples of the prediction points are within the bounds of the original training data. The variance values are relatively low.

- In this tutorial, variance (σ^2) is used to gauge the prediction uncertainty. Sometimes, you will see this prediction uncertainty expressed as the standard deviation (σ).



Response Surface

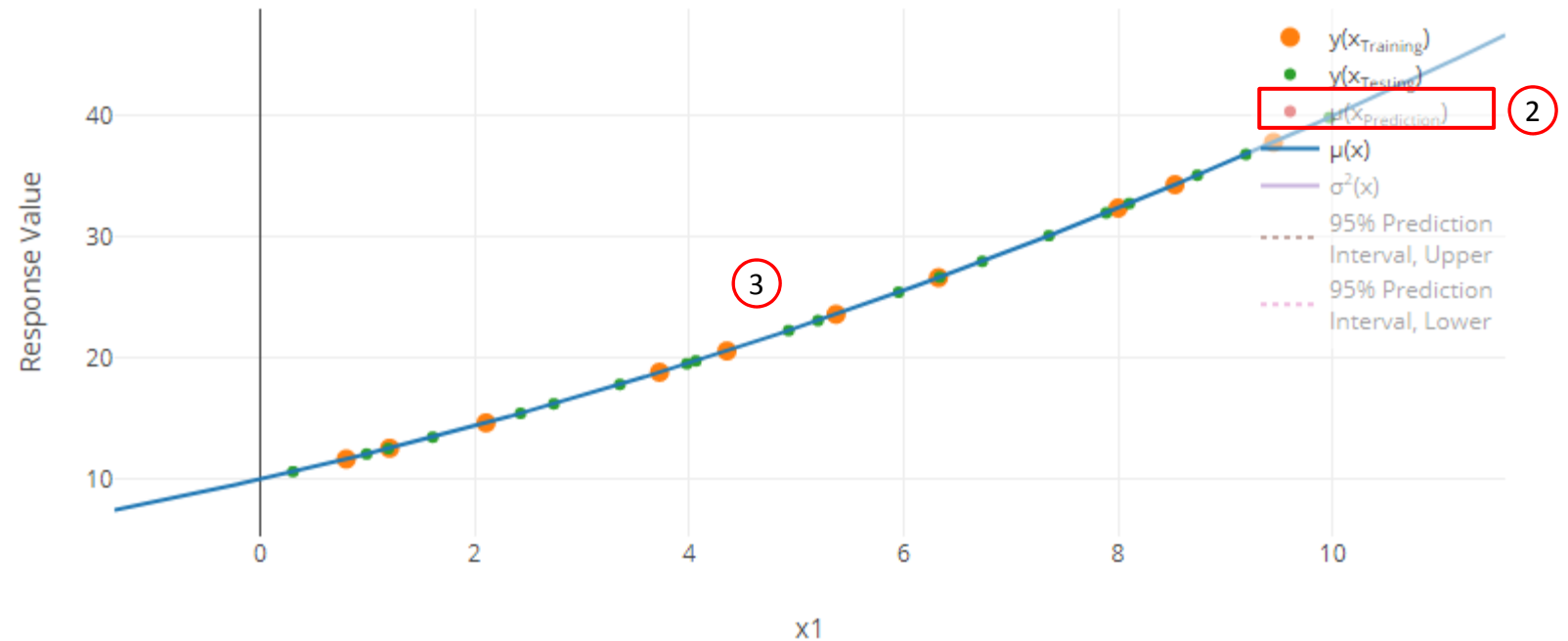
If the problem statement has 1 or 2 parameters configured, a response surface is created. For 3 or more parameters, a response surface is NOT created.

1. Navigate to the section titled Response Surface
2. Deselect the following legend entry:
 - $\mu(x_{\text{Prediction}})$
3. The plot is updated
 - $y(x_{\text{Training}})$: MSC Nastran responses used to train the surrogate model
 - $y(x_{\text{Testing}})$: MSC Nastran responses used to compute the NRMSE
 - $\mu(x_{\text{Prediction}})$: The predicted values at points $x_{\text{prediction}}$
 - $\mu(x)$: The predicted function

Regression Results

Response Surface ①

Matern52



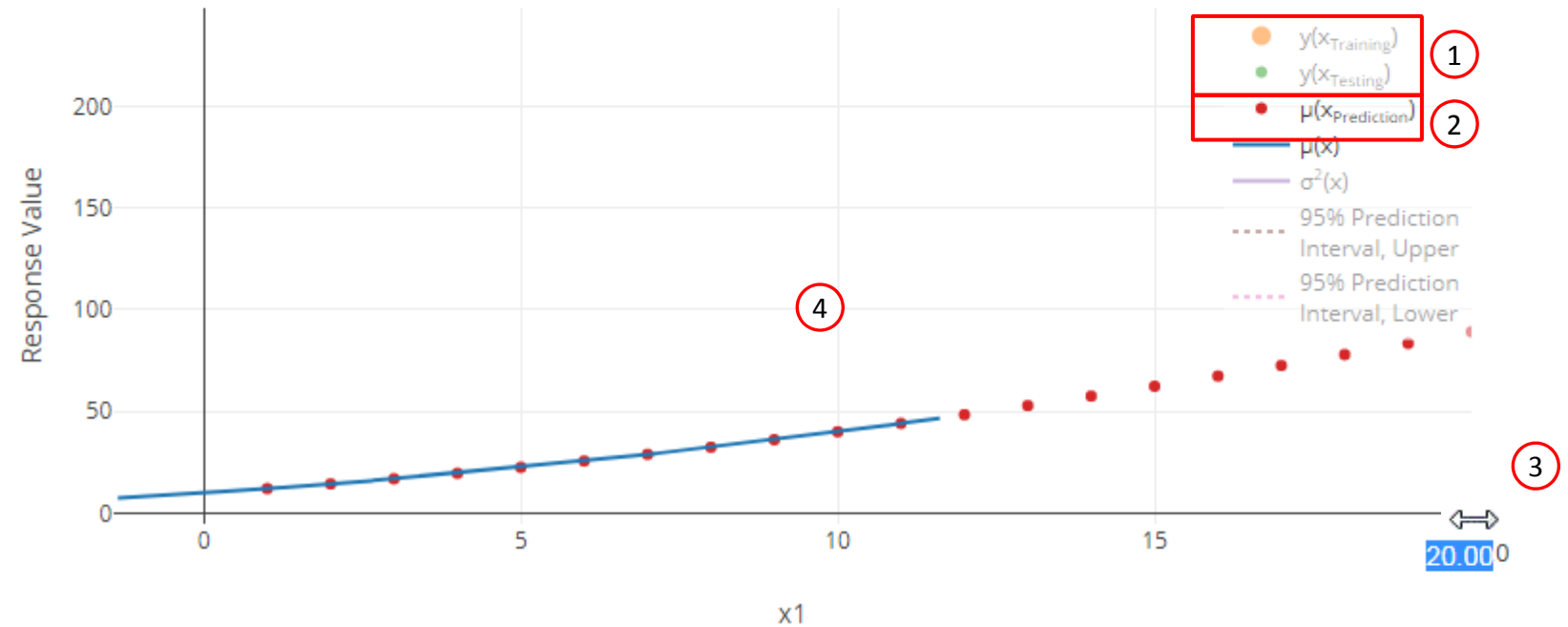
Response Surface

Matern52

Response Surface

1. Deselect the following legend entries
 - $y(x_{\text{Training}})$
 - $y(x_{\text{Testing}})$
2. Select the following legend
 - $\mu(x_{\text{Prediction}})$
3. Move the mouse cursor to the right most number label of the horizontal axis, single click the number, type in a value of 20.0, and press Enter. This will cause the horizontal axis to be scaled to be within 0 and 20.0.
4. The plot is updated

The training data used to train the surrogate model was within .1 and 10.0. Predictions should be made within these bounds. Predictions outside the bounds should NOT be performed.



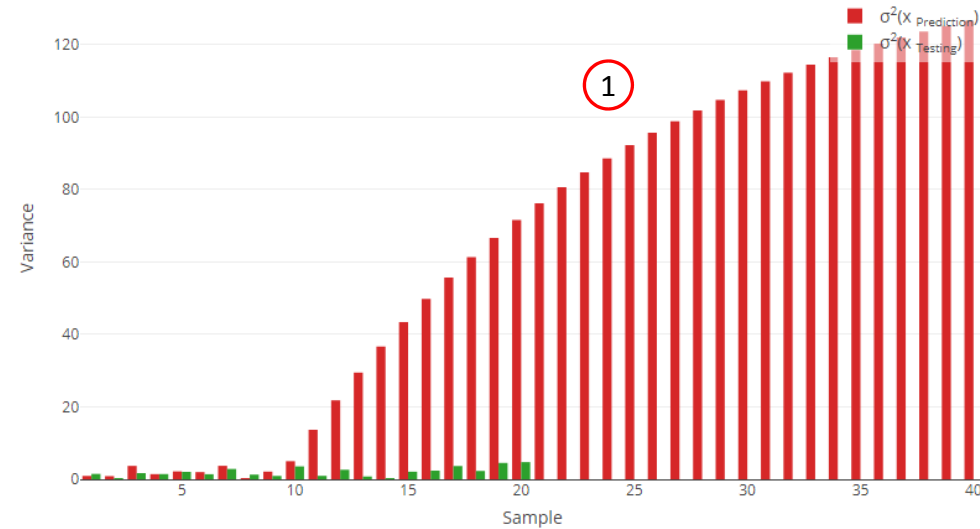
Response Surface

The training data used to train the surrogate model was within .1 and 10.0. Predictions should be made within these bounds. Predictions outside the bounds should NOT be performed.

1. The variance (prediction uncertainty) plot shows that the prediction uncertainty increases as you travel away from the bounds
2. To summarize
 - OK – Predictions are made within the bounds.
 - OK – Predictions are made close to the bounds. In some cases, the surrogate model has good prediction performance for points nearby the bounds.
 - NOT OK – Predictions are made far outside the bounds.

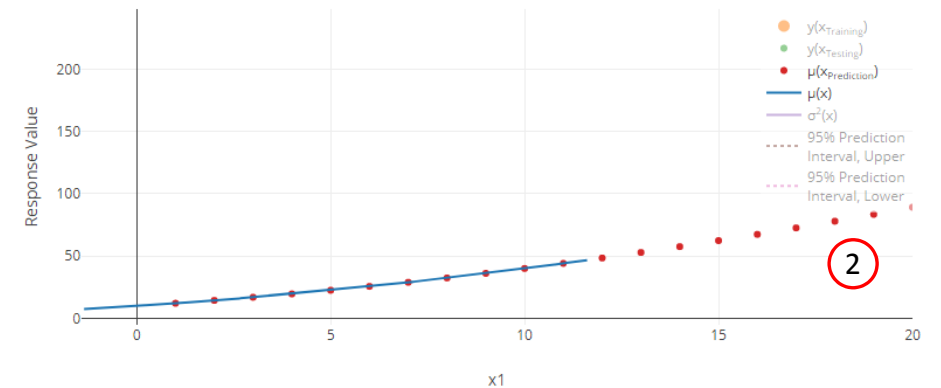
Exponential

NRMSE: 0.019861846267229557



Response Surface

Matern52



Creating Plots with the HDF5 Explorer

Start Desktop App

1. Open this folder:
nastran_working_directory
2. Inside of the new folder, double click on
Start Desktop App
3. Click Open, Run or Allow Access on any
subsequent windows

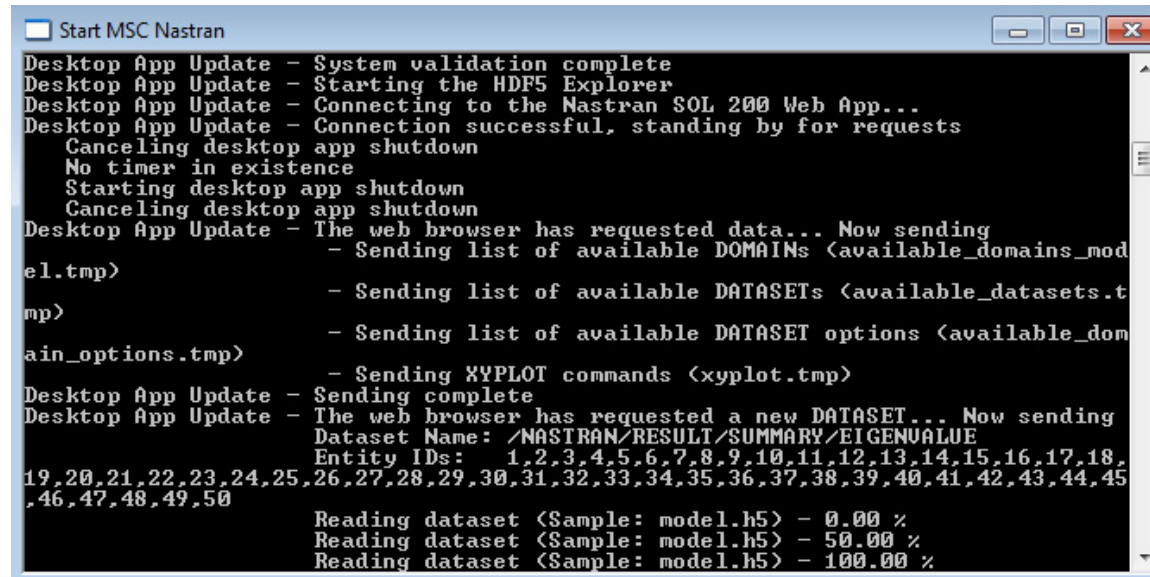
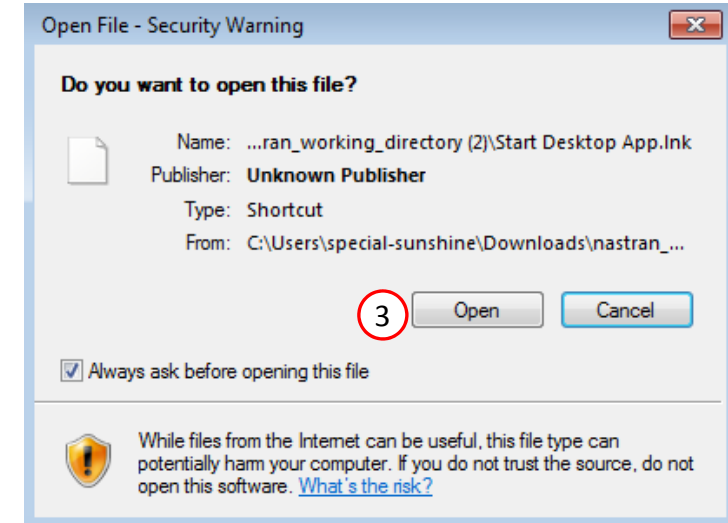
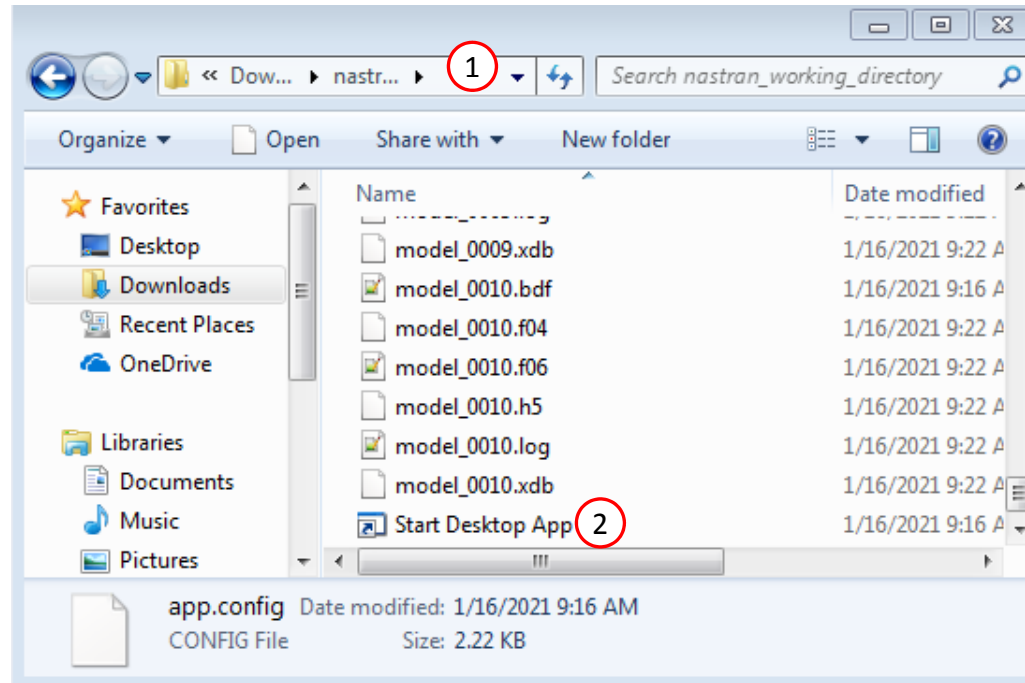
Using Linux?

Follow these instructions:

- 1) Open Terminal
- 2) Navigate to the nastran_working_directory
`cd ./nastran_working_directory`
- 3) Use this command to start the process
`./Start_MSC_Nastran.sh`

In some instances, execute permission must be granted to the directory. Use this command. This command assumes you are one folder level up.

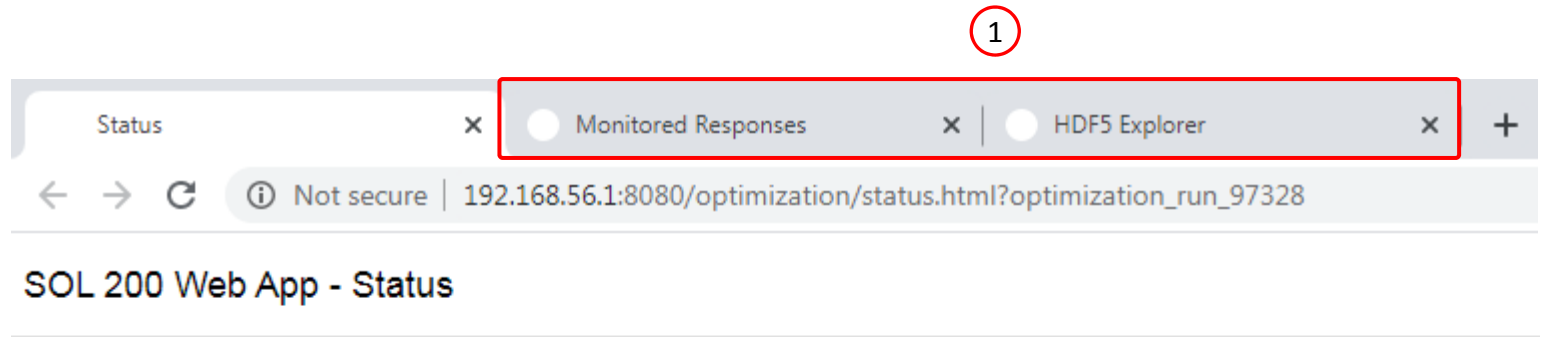
```
sudo chmod -R u+x ./nastran_working_directory
```



Results

Multiple web apps are automatically opened to display the results.

1. Use the tabs to switch between each web app
2. A description of each web app is given in the table.



Name of Web App	Purpose	Description
Monitored Responses	<ul style="list-style-type: none">• The response value from each sample can be compared.	<ul style="list-style-type: none">• After each MSC Nastran analysis, the response values are extracted from the H5 file and contained in a file named app_monitored_responses.csv. The Monitored Responses web app is used to create a bar chart of the values contained in this CSV file.
HDF5 Explorer	<ul style="list-style-type: none">• This web app is used to probe each H5 file and generate XY plots.	

Review Results

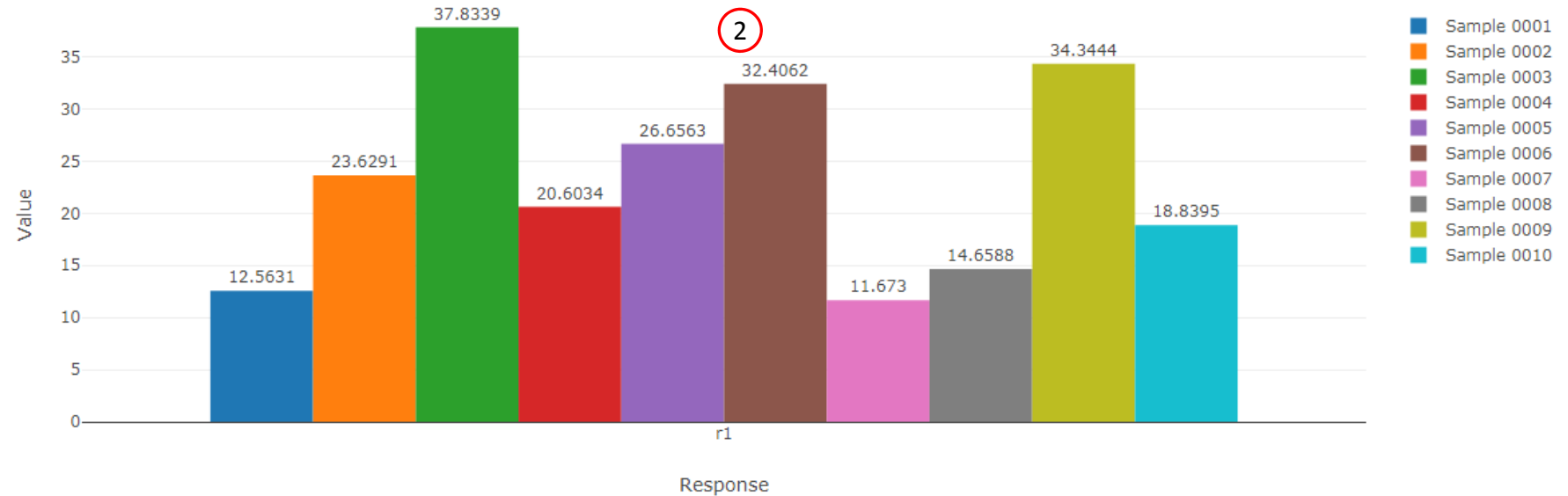
After MSC Nastran is finished, the results will be automatically uploaded.

1. On this page, the Monitored Responses web app is opened.
2. The value of each response and for each sample is displayed in a bar chart
3. A table lists the values for each response and sample.

A. Additional functions include the ability to highlight the MAX and MIN bars, download a CSV file and reset the filters.

SOL 200 Web App - Monitored Responses

Home



Monitored Responses

Display MAX and MIN Download CSV Reset Filters

Label	Dataset Name	Field	Field Description	Current Value
r1	SUMMARY/EIGENVALUE	EIGEN		
r1	SUMMARY/EIGENVALUE	EIGEN		10.001500337521877

Monitored Responses from Each Sample

0001	0002	0003	0004	
12.563078819847316	23.62907115939849	37.8338533140817	20.60335328534742	26.6563

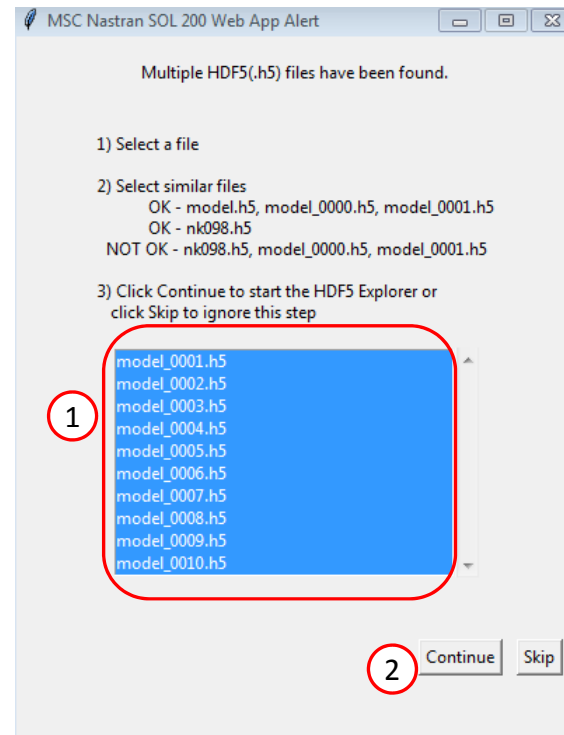
Review Results

On this page, the HDF5 Explorer is opened.

1. Select all the files
2. Click Continue
3. The HDF5 Explorer is automatically opened.
4. Click the image

The HDF5 Explorer is broken into sections.

- Acquire Dataset – Specific datasets from the H5 file can be extracted in this section.
- Plots Browser – Use this section to navigate every plot created.
- Combine Plots – This section allows you to combine multiple plots. For example, you can create Load vs. Displacement plots in this section.
- Last Plot Added – This display the last plot that was created.



SOL 200 Web App - HDF5 Explorer

3

Acquire Dataset

Plots Browser

Combine Plots

Last Plot Added

Plots Browser

SUMMARY/EIGENVALUE



Plot - SUMMARY/EIGENVALUE - Plot #: 0 - MODE: 1 | ORDER: 1 | SAMPLE: model_0001, model_0002, model_0003, ... | EIGEN vs. MODE



Vertical Axis



EIGEN -



2

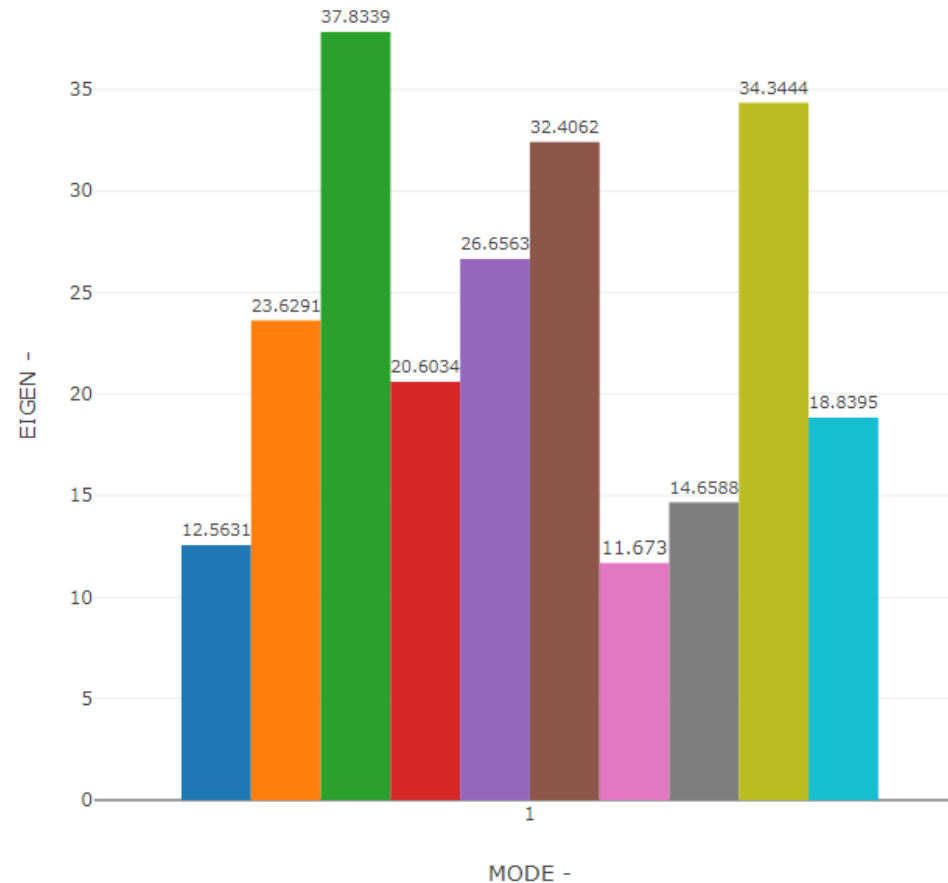
Horizontal Axis

MODE -

[+ Options](#)

SUMMARY/EIGENVALUE

1

☐ Display None ☒ Display All

Display	Color	Name
<input checked="" type="checkbox"/>	Blue	0 - MODE: 1 ORDER: 1 SAMPLE: model_0001
<input checked="" type="checkbox"/>	Orange	1 - MODE: 1 ORDER: 1 SAMPLE: model_0002
<input checked="" type="checkbox"/>	Green	2 - MODE: 1 ORDER: 1 SAMPLE: model_0003
<input checked="" type="checkbox"/>	Red	3 - MODE: 1 ORDER: 1 SAMPLE: model_0004
<input checked="" type="checkbox"/>	Purple	4 - MODE: 1 ORDER: 1 SAMPLE: model_0005
<input checked="" type="checkbox"/>	Brown	5 - MODE: 1 ORDER: 1 SAMPLE: model_0006
<input checked="" type="checkbox"/>	Pink	6 - MODE: 1 ORDER: 1 SAMPLE: model_0007
<input checked="" type="checkbox"/>	Grey	7 - MODE: 1 ORDER: 1 SAMPLE: model_0008
<input checked="" type="checkbox"/>	Yellow	8 - MODE: 1 ORDER: 1 SAMPLE: model_0009
<input checked="" type="checkbox"/>	Cyan	9 - MODE: 1 ORDER: 1 SAMPLE: model_0010

Review Results

1. After clicking on the image in the previous step, the respective plot is displayed. By default, a Frequency vs. Mode plot has been created. The plot display displays the 1st frequency for the samples.
2. An Eigenvalue vs. Mode plot is created by setting the vertical axis to EIGEN. The updated plot displays the 1st eigenvalue for the samples.

End of Tutorial

Appendix

Appendix Contents

- How to import and edit previous files
- What is Gaussian Process Regression?

How to import and edit previous files

How to import and edit previous files

The parameters, samples and responses are contained in the following files

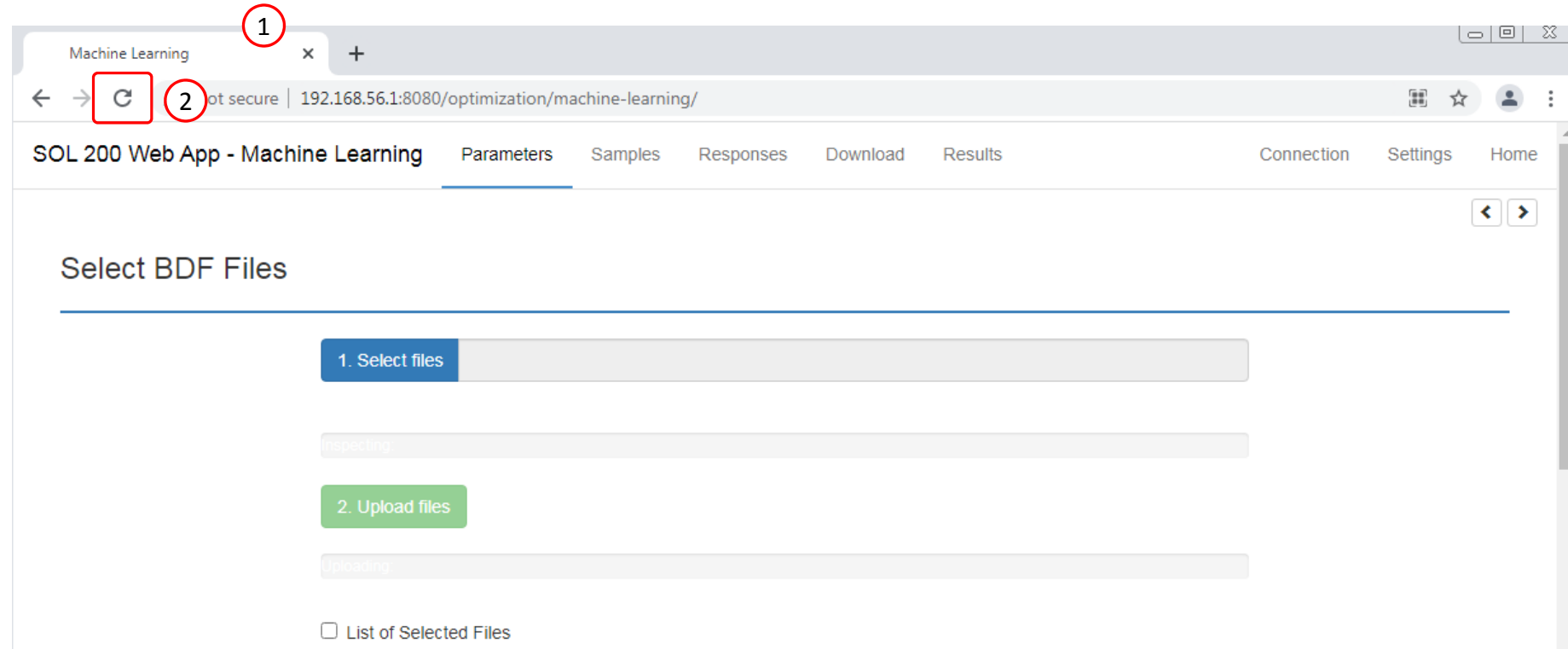
- app.config
- BDF files

These files may be imported back to the Parameter Study web app, and any parameters, samples and responses can be reconfigured

Import

1. Return to the window or tab that has the Parameter Study web app opened
2. Refresh the web page to start a new session

- Refreshing the page is only required when the *Select files* button is disabled.



Import

1. Click Select Files
2. Navigate to the folder named nastran_working_directory
3. Select all the BDF files AND the app.config file.
4. Click Open
5. Click Upload files

- All imports require the app.config file to be selected.

Select BDF Files

1. Select files 2 files selected

Inspecting: 100%

5. Upload files

Uploading

Open

« Downloads ▶ nastran_working_directory ▶ 2

Search nastran_working_direct...

Organize New folder

Name	Date modified	Type	Si
app	1/16/2021 9:16 AM	File folder	
temp_files_900	1/16/2021 12:06 PM	File folder	
app.config	1/16/2021 9:16 AM	CONFIG File	
model.bdf	1/16/2021 9:16 AM	BDF File	
model_0001.bdf	1/16/2021 9:16 AM	BDF File	
model_0002.bdf	1/16/2021 9:16 AM	BDF File	
model_0003.bdf	1/16/2021 9:16 AM	BDF File	
model_0004.bdf	1/16/2021 9:16 AM	BDF File	
model_0005.bdf	1/16/2021 9:16 AM	BDF File	
model_0006.bdf	1/16/2021 9:16 AM	BDF File	
model_0007.bdf	1/16/2021 9:16 AM	BDF File	
model_0008.bdf	1/16/2021 9:16 AM	BDF File	

File name: "model_0010.bdf" "app.config" "model.bdf" "model" 4

Custom Files (*.bdf;*.dat;*.conf)

Open Cancel

Import

For the Response section, the H5 file will need to be re-uploaded.

1. Click Responses
2. Select the H5 file
3. Click Upload
4. Data from the H5 is loaded and ready to use

SOL 200 Web App - Machine Learning Parameters Samples **Responses** Download Results Connection Settings Home

1

Upload .h5 File

2 1. Select files nas103_ws07_with_spring_support.h5

3 2. Upload files

Uploading

Loading

View Responses to Monitor

Monitored Responses Hide/Show Columns Reset Filters Download CSV

Delete	Label	Status	Objective	Lower Bound	Upper Bound	Monitor the of the FIN/ cycle (SOL
	r1			Lower	Upper	

SOL 200 Web App - Machine Learning Parameters Samples **Responses** Download Results Connection Settings Home

Select Responses to Monitor

Session ID: 6449 HDF5

Select Dataset

- ELEMENTAL/ELEMENT
- ELEMENTAL/ELEMENT
- NODAL/DISPLACEMENT
- NODAL/EIGENVECTOR
- SUMMARY/EIGENVALUE

Specify Entities

20

Element identification number (EID)
Examples: 20, etc.

☒ Auto Execute

Acquire Dataset

Acquisition complete and successful

Acquired Dataset

ELEMENTAL/ELEMENT_FORCE/ELAS1 - 20

EID	F	SAMPLE	DOMAIN_ID
Element identification number	User defined	Name of H5 File**	Domain identifier
20		nas103	
20	-0.00010000...	nas103_...	1
20	0.001	nas103_...	3

4

View Responses to Monitor

Monitored Responses Hide/Show Columns Reset Filters Download CSV

Delete	Label	Status	Objective	Lower Bound	Upper Bound	Monitor the of the FIN/ cycle (SOL
	r1			Lower	Upper	

5 10 20 30 50 100

Import

After import, any Parameter, Samples or Responses can be modified.



Select BDF Files

1. Select files

2 files selected

Inspecting: 100%

2. Upload files

Uploading: 100 %

☐ List of Selected Files

Select Parameters

\$ _1 _ || _2 _ || _3 _ || _4 _ || _5 _ || _6 _ || _7 _ || _8 _ || _9 _ || _10 _ |

EIGB	30	INV	0.	3.	20	2	2
FORCE	6	2		1.	0.	-1.	0.
MAT1	1	10.E7					
PELAS	20	%x1%					
PROD	10	1	.1				

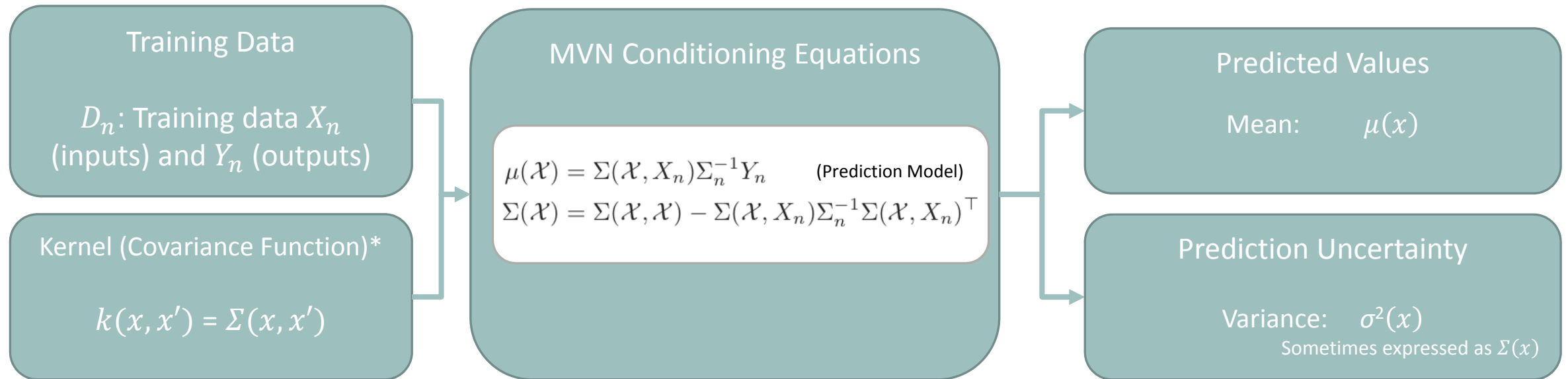


Configure Parameters

Delete	Parameter	Status	Low	High	Comments
	x1		.1	10.	Field 3 of PELAS

What is Gaussian Process Regression?

Gaussian Process Regression Overview



* Hyperparameter optimization is part of the procedure but not covered in this presentation

** $\mu(x)$: This function corresponds to the mean function or kriging model. This function is the prediction model, also known as the surrogate model, meta model or emulator.

Multivariate Normal (MVN) Conditioning Equations

The following must be calculated: Covariance Matrix, Mean and Variance

Covariance Matrix

$$\Sigma = \begin{pmatrix} \Sigma(\chi, \chi) & \Sigma(\chi, X_n) \\ \Sigma(X_n, \chi) & \Sigma_n = \Sigma(X_n, X_n) \end{pmatrix}$$

X_n : Training locations
 χ : Testing (predictive) locations

Apply the covariance function $\Sigma(x, x')$ (kernel $k(x, x')$)

- $\Sigma(\chi, \chi)$: Covariance between testing (predictive) locations and themselves
- $\Sigma(\chi, X_n)$: Covariance between testing (predictive) and training locations
- $\Sigma(X_n, \chi)$: Covariance between training and testing (predictive) locations, which is the transpose of $\Sigma(\chi, X_n)$
- $\Sigma_n = \Sigma(X_n, X_n)$: Covariance between training locations and themselves

MVN Conditioning Equations (Mean and Variance)

Also referred to as “Gaussian process regression,” “kriging” or “kriging equations”

mean $\mu(\chi) = \Sigma(\chi, X_n) \Sigma_n^{-1} Y_n$ Prediction Model (Vary χ to make predictions)

and variance $\Sigma(\chi) = \Sigma(\chi, \chi) - \Sigma(\chi, X_n) \Sigma_n^{-1} \Sigma(X_n, \chi)^T$ Prediction Uncertainty

Example 1

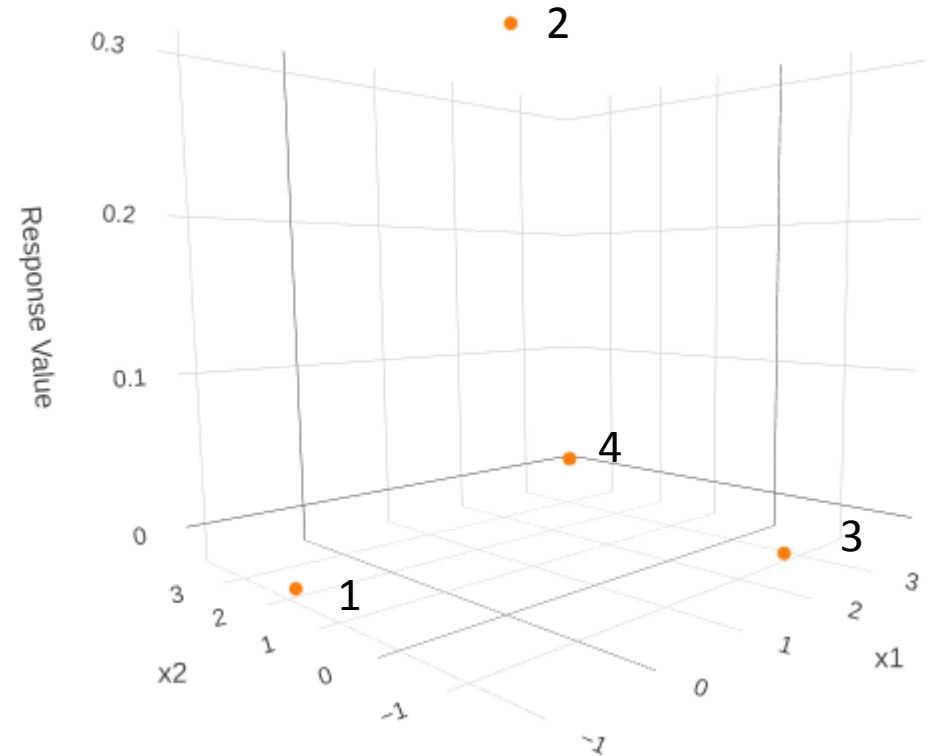
Example 1

Suppose a black box function was executed at 4 different samples (x1, x2 combinations)

With limited data (x and y), what does the response surface look like?

Training Data

Sample	x1	x2	y
1	-1.03	1.76	-1.56E-02
2	.49	.49	3.04E-01
3	1.77	-1.77	3.38E-03
4	3.62	3.76	5.43E-12



Training Data and Testing (Predictive) Locations

Suppose you have the following training data (X_n and Y_n) and testing locations (χ)

- X_n : The training design consists of 4 points
- χ : The test design (locations to make predictions) consists of 2 points

$$X = \begin{bmatrix} \chi \\ X_n \end{bmatrix} = \begin{bmatrix} .35 & .69 \\ .65 & .46 \\ -1.03 & 1.76 \\ .49 & .49 \\ 1.77 & -1.77 \\ 3.62 & 3.76 \end{bmatrix}$$

$$\begin{bmatrix} y^* \\ Y_n \end{bmatrix} = \begin{bmatrix} ? \\ ? \\ -1.56e-02 \\ 3.04e-01 \\ 3.38e-03 \\ 5.43e-12 \end{bmatrix}$$

The goal is make predictions (y^*) for points in χ

Note

- X_n : inputs of the training data
- Y_n : outputs of the training data
- χ or x : inputs of the testing data (predictive locations, i.e. points to make predictions)
- y^* : predicted outputs
- D_n : Training data X_n and Y_n

X : upper case of Greek letter chi (pronounced kai in English)
 χ : lower case of Greek letter chi

Calculation of the Covariance Matrix

1. Select a covariance (kernel) function

- Many covariance functions (kernels) exist: Radial Basis Function (RBF), Matern 5/2, 3/2, Exponential, ...
- For this example, a form of the RBF covariance function is used. This covariance function is described as the “inverse exponentiated squared Euclidean distance”

$$k(x, x') = \Sigma(x, x') = \exp\{-\|x - x'\|^2\} = e^{-\|x - x'\|^2}$$

2. Calculate D (Distance Matrix)

$$D = \|X - X\|^2 \quad \text{“Norm between } X \text{ and } X, \text{ squared”}$$

3. Calculate Σ (Covariance Matrix)

$$\Sigma = e^{-D}$$

Calculation of D

$D =$

$\sqrt{(.35 - .35)^2 + (.69 - .69)^2}$ = 0	$\sqrt{(.35 - .65)^2 + (.69 - .46)^2}$ = .1429	$\sqrt{(.35 - -1.03)^2 + (.69 - 1.76)^2}$ = 3.0493	$\sqrt{(.35 - .49)^2 + (.69 - .49)^2}$ = .0596	$\sqrt{(.35 - 1.77)^2 + (.69 - -1.77)^2}$ = 8.068	$\sqrt{(.35 - 3.62)^2 + (.69 - 3.76)^2}$ = 20.1178
.1429	$\sqrt{(.65 - .65)^2 + (.46 - .46)^2}$ = 0	$\sqrt{(.65 - -1.03)^2 + (.46 - 1.76)^2}$ = 4.5124	$\sqrt{(.65 - .49)^2 + (.46 - .49)^2}$ = .0265	$\sqrt{(.65 - 1.77)^2 + (.46 - -1.77)^2}$ = 6.2273	$\sqrt{(.65 - 3.62)^2 + (.46 - 3.76)^2}$ = 19.7109
3.0493	4.5124	$\sqrt{(-1.03 - -1.03)^2 + (1.76 - 1.76)^2}$ = 0	$\sqrt{(-1.03 - .49)^2 + (1.76 - .49)^2}$ = 3.9233	$\sqrt{(-1.03 - 1.77)^2 + (1.76 - -1.77)^2}$ = 20.3009	$\sqrt{(-1.03 - 3.62)^2 + (1.76 - 3.76)^2}$ = 25.6225
.0596	.0265	3.9233	$\sqrt{(.49 - .49)^2 + (.49 - .49)^2}$ = 0	$\sqrt{(.49 - 1.77)^2 + (.49 - -1.77)^2}$ = 6.746	$\sqrt{(.49 - 3.62)^2 + (.49 - 3.76)^2}$ = 20.4898
8.068	6.2273	20.3009	6.746	$\sqrt{(1.77 - 1.77)^2 + (-1.77 - -1.77)^2}$ = 0	$\sqrt{(1.77 - 3.62)^2 + (-1.77 - 3.76)^2}$ = 34.0034
20.1178	19.7109	25.6225	20.4898	34.0034	$\sqrt{(3.62 - 3.62)^2 + (3.76 - 3.76)^2}$ = 0

Calculation of Σ

$$\Sigma = \begin{bmatrix} e^0 = 1 & e^{-.1429} = .8668 & e^{-3.0493} = .0474 & e^{-.0596} = .9421 & e^{-8.068} = .0003 & e^{-20.1178} = 1.832e-9 \\ .8668 & e^0 = 1 & e^{-4.5124} = .0110 & e^{-.0265} = .9738 & e^{-6.2273} = .0020 & e^{-19.7109} = 2.8e-9 \\ .0474 & .0110 & e^0 = 1 & e^{-3.9233} = .0198 & e^{-20.3009} = 1.5e-9 & e^{-25.6225} = 7.5e-12 \\ .9421 & .9738 & .0198 & e^0 = 1 & e^{-6.746} = .0012 & e^{-20.4898} = 1.263e-9 \\ .0003 & .0020 & 1.5e-9 & .0012 & e^0 = 1 & e^{-34.0034} = 1.7e-15 \\ 1.832e-9 & 2.8e-9 & 7.5e-12 & 1.263e-9 & 1.7e-15 & e^0 = 1 \end{bmatrix}$$

Calculation of Σ

$\Sigma =$

$$\Sigma(\chi, \chi)$$

$e^0 = 1$	$e^{-1429} = .8668$
$.8668$	$e^0 = 1$

$$\Sigma(\chi, X_n)$$

$e^{-3.0493} = .0474$	$e^{-.0596} = .9421$	$e^{-8.068} = .0003$	$e^{-20.1178} = 1.832e-9$
$e^{-4.5124} = .0110$	$e^{-.0265} = .9738$	$e^{-6.7273} = .0020$	$e^{-19.7109} = 2.8e-9$

$$\Sigma(X_n, \chi)$$

$.0474$	$.0110$
$.9421$	$.9738$
$.0003$	$.0020$
$1.832e-9$	$2.8e-9$

$$\Sigma_n = \Sigma(X_n, X_n)$$

$e^0 = 1$	$e^{-3.9233} = .0198$	$e^{-20.3009} = 1.5e-9$	$e^{-25.6225} = 7.5e-12$
$.0198$	$e^0 = 1$	$e^{-6.746} = .0012$	$e^{-20.4893} = 1.263e-9$
$1.5e-9$	$.0012$	$e^0 = 1$	$e^{-34.0034} = 1.7e-15$
$7.5e-12$	$1.263e-9$	$1.7e-15$	$e^0 = 1$

Since Σ is symmetric, note that $\Sigma(X_n, \chi) = \Sigma(\chi, X_n)^T$

Calculation of Predictive Quantities

The MVN conditioning equations are used to determine the predictive quantities mean and variance

mean $\mu(\mathcal{X}) = \Sigma(\mathcal{X}, X_n) \Sigma_n^{-1} Y_n$

$$\mu(\chi) = y * = \begin{pmatrix} 0.2849657 \\ 0.2954011 \end{pmatrix} \quad \text{Predicted values for locations in } \chi$$

and variance $\Sigma(\mathcal{X}) = \Sigma(\mathcal{X}, \mathcal{X}) - \Sigma(\mathcal{X}, X_n) \Sigma_n^{-1} \Sigma(\mathcal{X}, X_n)^\top$

$$\Sigma(\chi) = \begin{pmatrix} 0.11154162 & -0.05042265 \\ -0.05042265 & 0.05155061 \end{pmatrix} \quad \text{Prediction Uncertainty}$$

The diagonal terms are the variances at prediction points 1 and 2

$$\sigma^2(\chi) = \begin{pmatrix} 0.11154162 \\ 0.05155061 \end{pmatrix}$$

R

Code to replicate this example in R

```
library(plgp)

eps = sqrt(.Machine$double.eps)

# Training points
X = rbind(c(-1.03,1.76), c(.49,.49), c(1.77,-1.77), c(3.62,3.76))

# The goal is to fit this function:  $y(x) = x_1 * \exp(-x_1^2 - x_2^2)$ 
y = X[,1] * exp(-X[,1]^2 - X[,2]^2)

# Test points
XX = rbind(c(.35, .69), c(.65, .46))
XX

# Sigma 22 (Sigma) and its inverse (Si)
# #####
# Distance among the Training Data
D = distance(X)
Sigma = exp(-D)
Si = solve(Sigma)

# Sigma 11
# #####
# Distance among the Testing Data
DXX = distance(XX)
SXX = exp(-DXX)

# Sigma 12 and Sigma 21 (Transpose of Sigma 12)
# #####
# Distance between training and testing data
```

```
DX = distance(XX, X)
SX = exp(-DX)

# Calculate the predictive mean and predictive variance
# #####
# Predictive mean
mup = SX %*% Si %*% y
mup

# Predictive variance
Sigmap = SXX - SX %*% Si %*% t(SX)
Sigmap
```

Output

```
> # #####
> # Predictive mean
> mup = SX %*% Si %*% y
> mup
      [,1]
[1,] 0.2849657
[2,] 0.2954011
>
> # Predictive variance
> Sigmap = SXX - SX %*% Si %*% t(SX)
> Sigmap
      [,1] [,2]
[1,] 0.11154162 -0.05042265
[2,] -0.05042265 0.05155061
>
```

R

Code to replicate this example in R with Plots

```
library(plgp)
library(lhs)

eps = sqrt(.Machine$double.eps)

# Training Data
# #####
# Training points
number_of_sample_points = 4
X = rbind(c(-1.03,1.76), c(.49,.49), c(1.77,-1.77), c(3.62,3.76))

# Observed values
# The goal is to fit this function:  $y(x) = x_1 * \exp(-x_1^2 - x_2^2)$ 
y = X[,1] * exp(-X[,1]^2 - X[,2]^2)

# Testing Data
# #####
# Test points
number_of_test_points_per_axis = 40
xx = seq(-2, 4, length=number_of_test_points_per_axis)
XX = expand.grid(xx, xx)

# Sigma 22 (Sigma) and its inverse (Si)
# #####
# Distance among the Training Data
D = distance(X)
Sigma = exp(-D) + diag(eps, nrow(X))
Si = solve(Sigma)

# Sigma 11
# #####
# Distance among the Testing Data
```

```
DXX = distance(XX)
SXX = exp(-DXX)

# Sigma 12 and Sigma 21 (Transpose of Sigma 12)
# #####
# Distance between training and testing data
DX = distance(XX, X)
SX = exp(-DX)

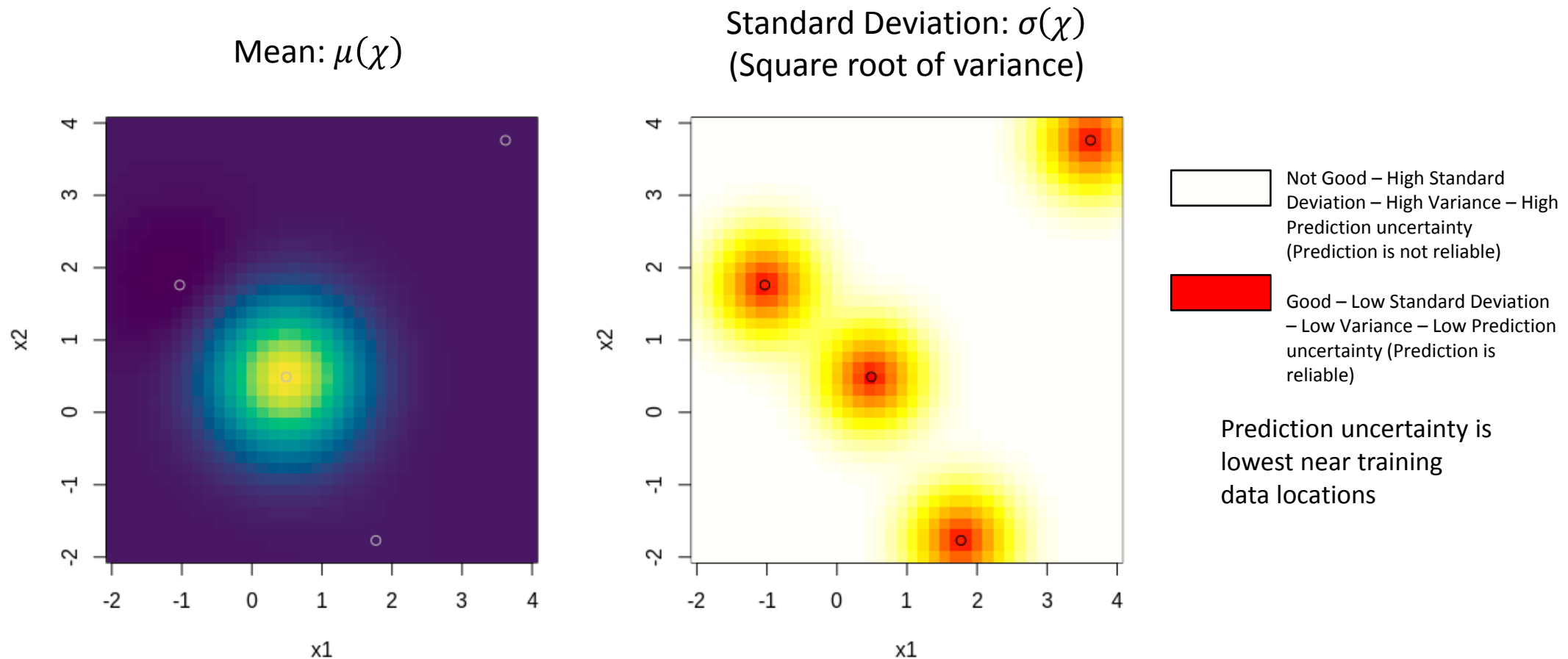
# Calculate the predictive mean and predictive variance
# #####
mup = SX %*% Si %*% y
Sigmap = SXX - SX %*% Si %*% t(SX)

# Predictive standard deviation
diag(Sigmap)
sdp = sqrt(diag(Sigmap))

# Figure 5.5
par(mfrow=c(1, 2))
cols_a = hcl.colors(128, palette = "viridis")
cols_b = heat.colors(128)
image(xx, xx, matrix(mup, ncol=length(xx)), xlab='x1', ylab='x2', col=cols_a)
points(X[,1], X[,2])
image(xx, xx, matrix(sdp, ncol=length(xx)), xlab='x1', ylab='x2', col=cols_b)
points(X[,1], X[,2])

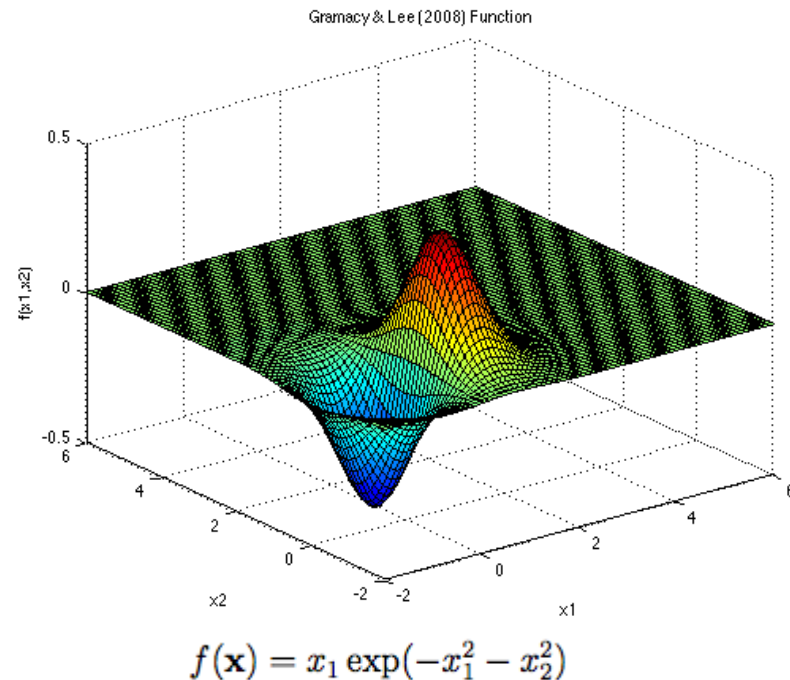
# Figure 5.6
persp(xx, xx, matrix(mup, ncol=number_of_test_points_per_axis), theta=-30, phi=30,
xlab='x1', ylab='x2', zlab='y', zlim = c(-.5,.5))
```

Predictive Quantities Mean and Standard Deviation



Comparison of True Function and Prediction Model

True Function



Source: <https://www.sfu.ca/~ssurjano/grlee08.html>

Prediction Model ($\mu(\chi)$)

