Reduced Order Models (ROMs) and RAVEN

RAVEN Workshop

PSA 2015 - April 26th 2015, Sun Valley (ID)

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Idaho National Laboratory

Outline

- Brief introduction on ROMs
- Application examples of ROMs
- ROMs and RAVEN
  - Available ROMs
  - RAVEN ROM workflow
- RAVEN examples
  - Create ROMs
  - Perform sampling of ROMs

ROMs: a Quick Introduction

- Consider a set of *N* data points

DataObjects (TimePointSet)

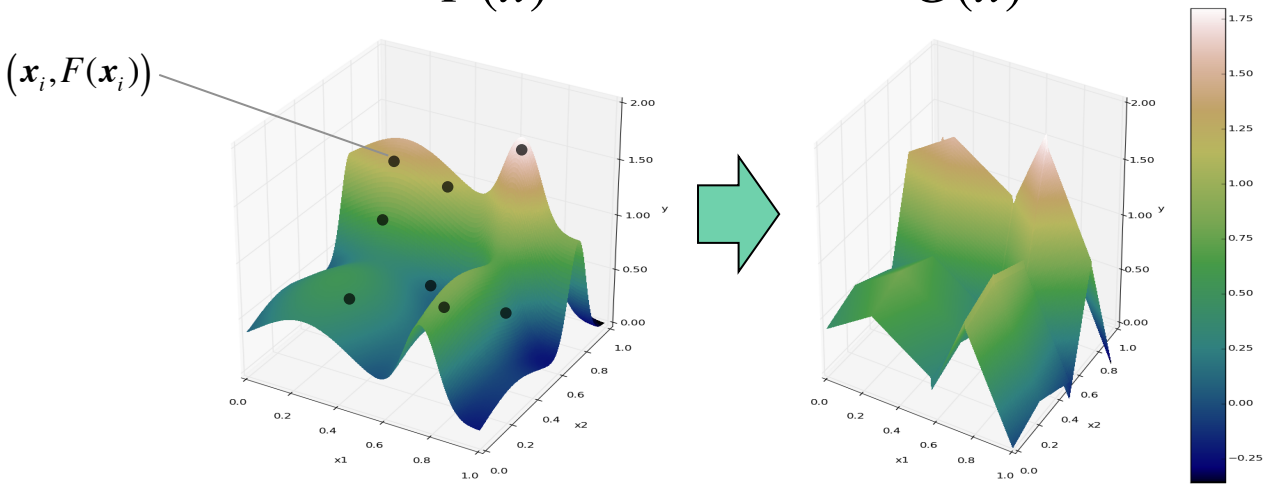
$$\left(x_i, F(x_i)\right) \quad i = 1,\ldots,N$$

Output: Simulation outcome (success/failure, max clad temperature)

Inputs: Initial and boundary conditions

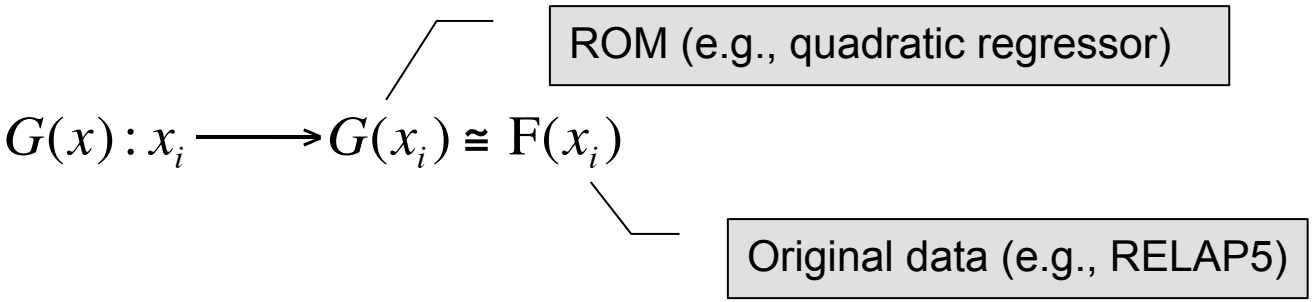
- Build a surrogate model
  - Reduced Order Model $G(x): x_i \longrightarrow G(x_i) \cong \mathrm{F}(x_i)$

$F(x)$ $G(x)$



ROMs: a Quick Introduction

- Basically we are trying to reduce the complexity of the original model



- Pros:
  - Much faster computation of the output variable
- Cons:
  - Presence of error in the ROM computed values

Classes of ROMs

- Model-Based
  - Prediction is performed using a blend of interpolation and regression algorithms
  - Examples:
    - Gaussian Process Models (GPMs)
    - Spline interpolator

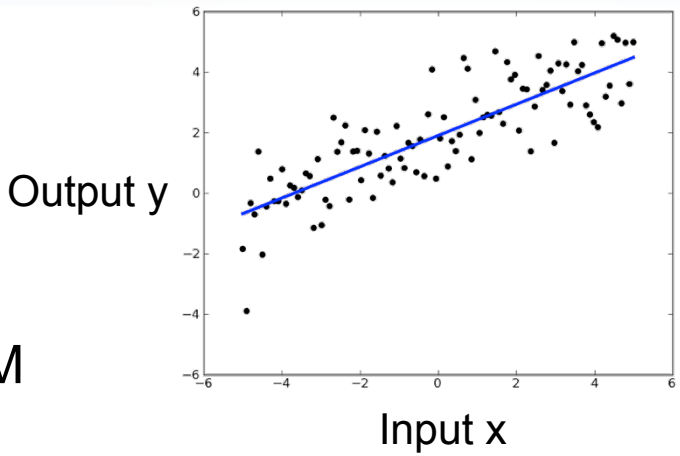
- Data-Based
  - Prediction is performed by solely considering the input data by using data searching algorithms
  - Examples:
    - Nearest neighbor

ROMs: Applications

- Basic steps:
  1. Sample original model
  2. Train the ROM

$$y = mx + c$$

  3. Perform desired analysis with the ROM instead of the original model



- Range of applications:
  - Uncertainty quantification / Sensitivity analysis
  - Probabilistic Risk Analysis (PRA)
  - Accelerator for stochastic analysis (adaptive sampling)
  - Prediction models

ROMs Available in RAVEN

- External libraries: Scikit-learn (http://scikit-learn.org)
  - Open source machine learning library for `Python`
  - Library for data mining and data analysis
  - Built on `NumPy` and `SciPy`

- Internally `C++` developed libraries: CROW
  - Generalized Polynomial Chaos
  - Multi-dimensional interpolators
    - ND Spline
    - ND Inverse-Weight

Scikit-Learn Library

- Available:
  - Classification: identifying to which category an object belongs
  - Regression: predicting a continuous-valued attribute
  - Data clustering: grouping similar objects into sets
  - Dimensionality reduction: reducing the number of random variables
  - Data pre-processing: feature extraction and normalization

- Examples:
  - Linear regression models
  - Support Vector Machines
  - Multi-Class classifiers
  - Naïve Bayes
  - Neighbors classifiers
  - Tree classifiers

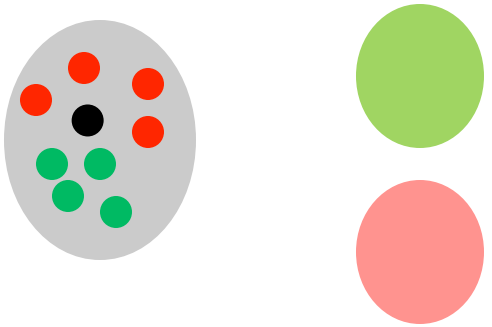
scikits learn
machine learning in Python

Scikit-Learn Library

- Classification
  - Starting point: set of data points with labels

    $[\text{features, class}]_i$

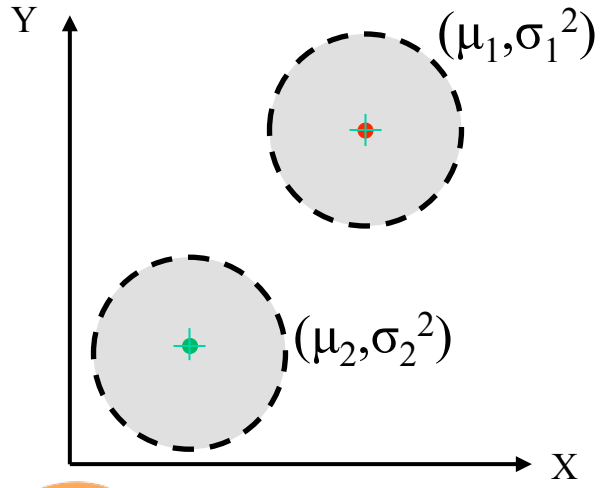
  - Objective: identify which class a new point [features] belong



- Clustering
  - Starting point: set of data points

    $[\text{features}]_i$

  - Objective: group data points based on a specific distance metrics



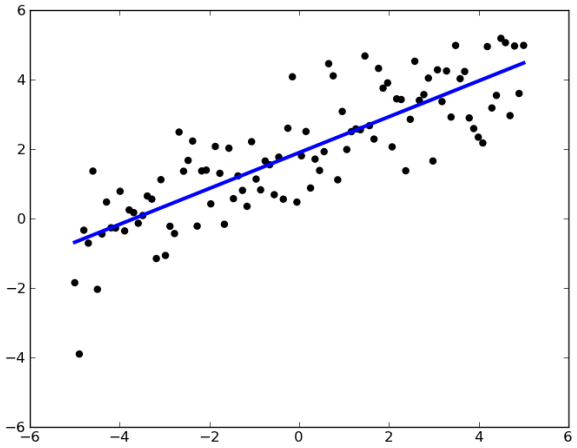
scikits learn
machine learning in Python

Scikit-Learn Library

Starting point: set of data points

$[\text{features}]_i$

- Cardinality reduction
  - Objective: identify the most relevant features that keep data points unique
  - Outcome: Location of the points on the reduced space (e.g., line)



Source: scikit-learn.org

- Regression
  - Objective: estimate the relationships among variables via a statistical process
  - Outcome: coefficients of the reduced space (e.g., *m* and *c* for linear interpolator $y = mx + c$)

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machine learning in Python

Generalized Polynomial Chaos

- Objective: overcome limitations of Monte-Carlo sampling
  - High number of samples
  - Computationally expensive

- Polynomial representation of an output variable $\Phi_k(Y)$
  - Simpler to evaluate
  - Easy to get statistical moments
  - Less effort and more accurate than Monte Carlo

$$u(Y) \approx \sum_{k \in \Lambda(L)} u_k \Phi_k(Y)$$

$$\Phi_k(Y) = \prod_{n=1}^{N} \Phi_{k_n}^{(n)}(y_n)$$

index set of all desired polynomial orders up to order L

Multi-Dimensional Interpolators

- CROW: Internally developed C++ library
- Interpolation on any dimension
- Response surface is created as an interpolation function given a set of data points defined on:
  - Sparse grid
  - Cartesian grid
- Extension of the known 1-D interpolation schemes

Multi-Dimensional Interpolators

- Two classes of algorithms
  1. Inverse-Weight
     - No interpolation kernel is defined
     - Defined on sparse grid

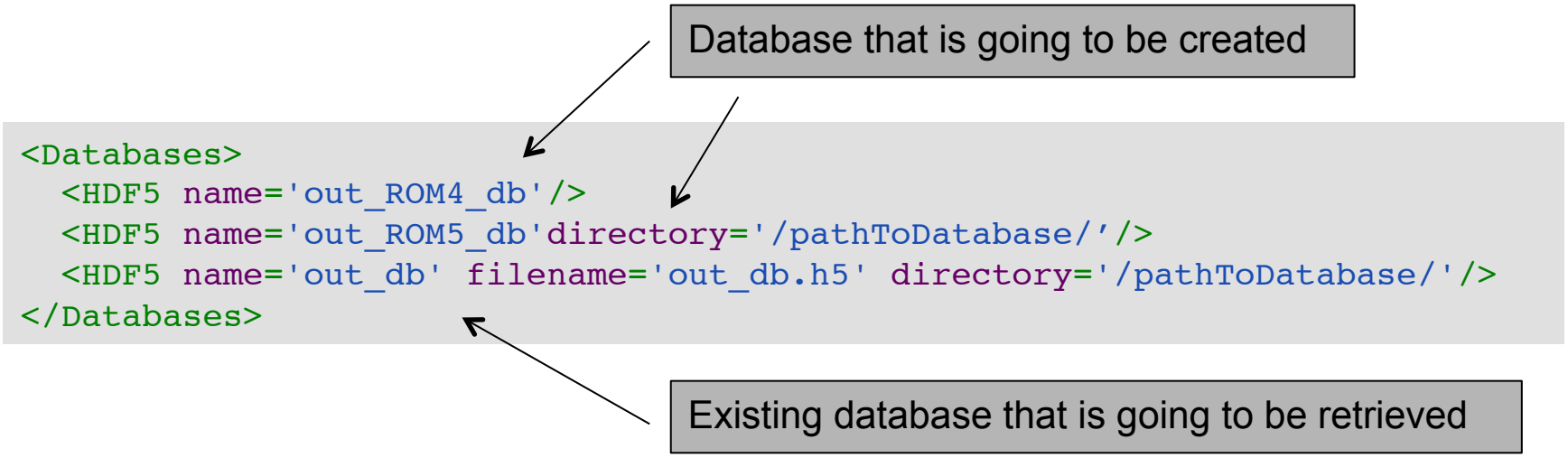
$$u(x) = \begin{cases} \dfrac{\sum_{i=1}^{N} w_i(x) \cdot u_i}{\sum_{i=1}^{N} w_i(x)} & d(x_i, x) \neq 0 \\ u_i & d(x_i, x) = 0 \end{cases}$$

where: $w_i(x) = \dfrac{1}{d(x_i, x)^P}$

  2. Multi-Dimensional Spline
     - Defined on cartesian grid
     - Based on multi-dimensional spline kernel
     - Continuity of the derivative is preserved

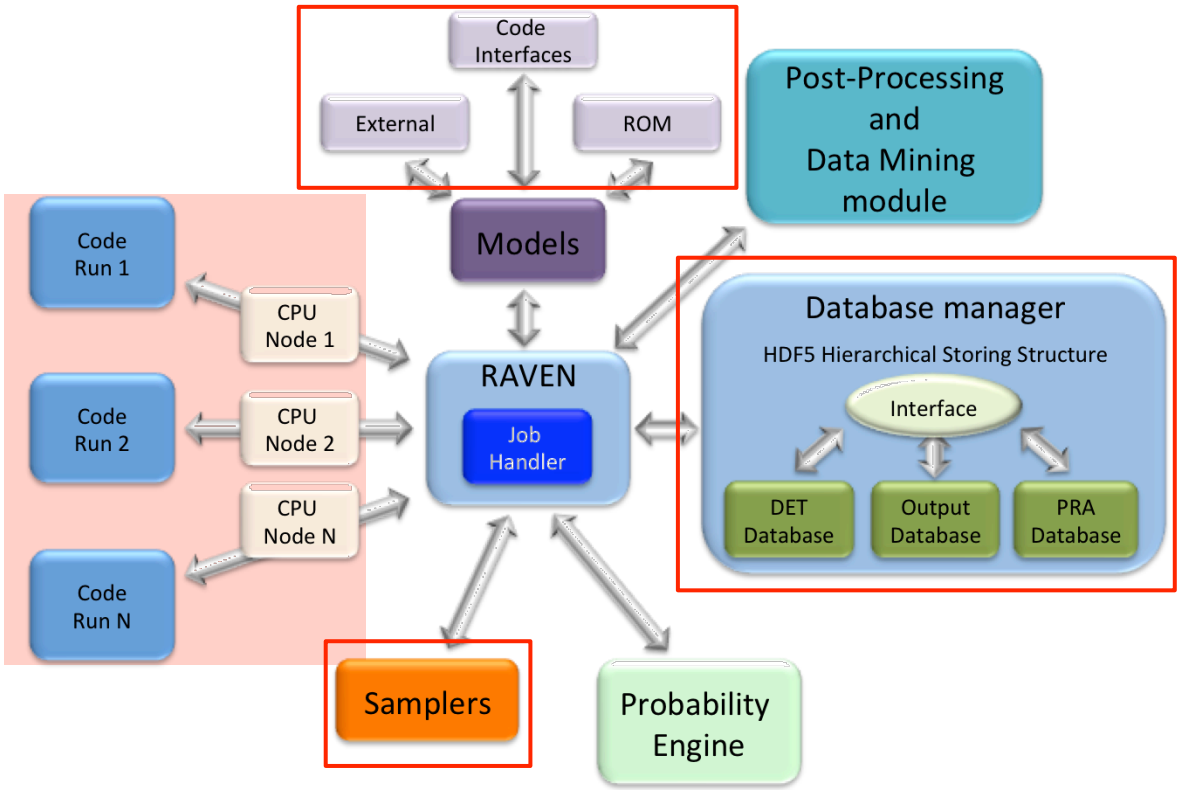
Database Storage in RAVEN

- RAVEN framework provides the capability to store and retrieve data to/ from an external database
- Database format: HDF5
- Data can be organized in two ways:
  - Parallel (e.g., if generated from a Monte-Carlo sampler)
  - Hierarchical (e.g., if generated from a Dynamic Event Tree sampler)



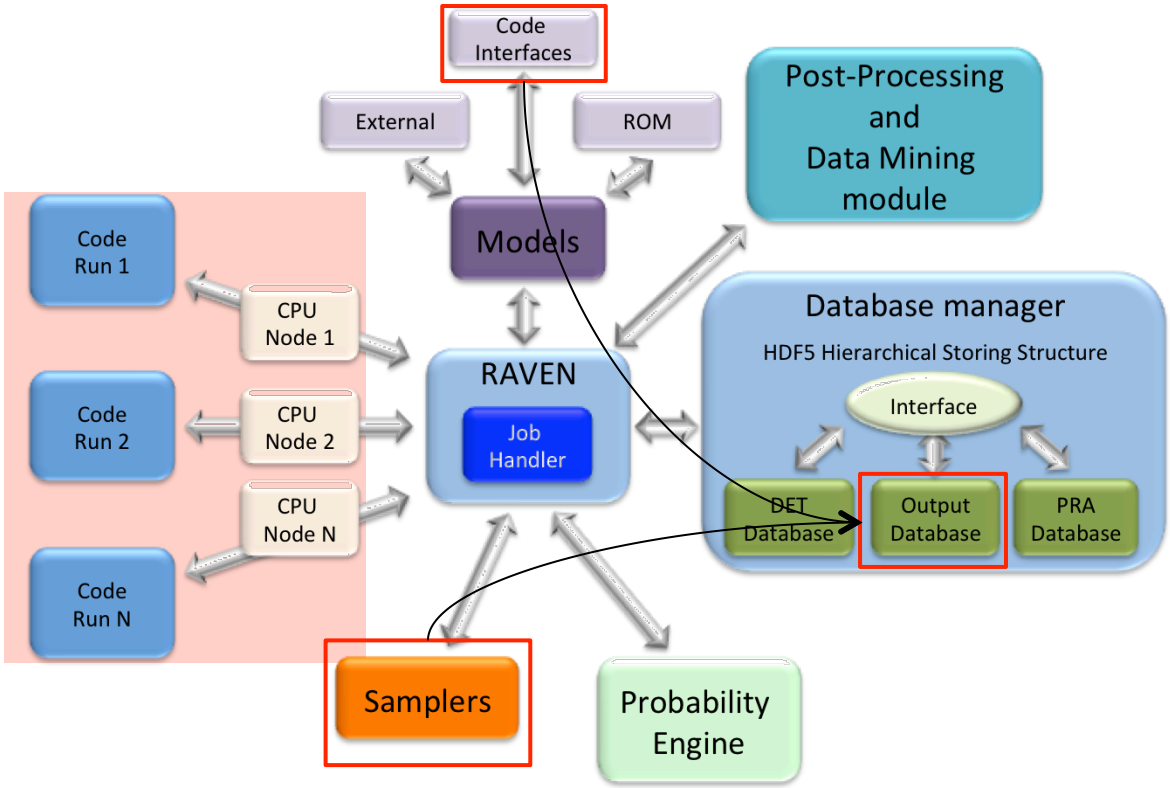
ROM Modeling Within RAVEN

- All modeling steps that involve ROMs are available in RAVEN
  - Create ROMs from a database
  - Perform statistical analysis using ROMs



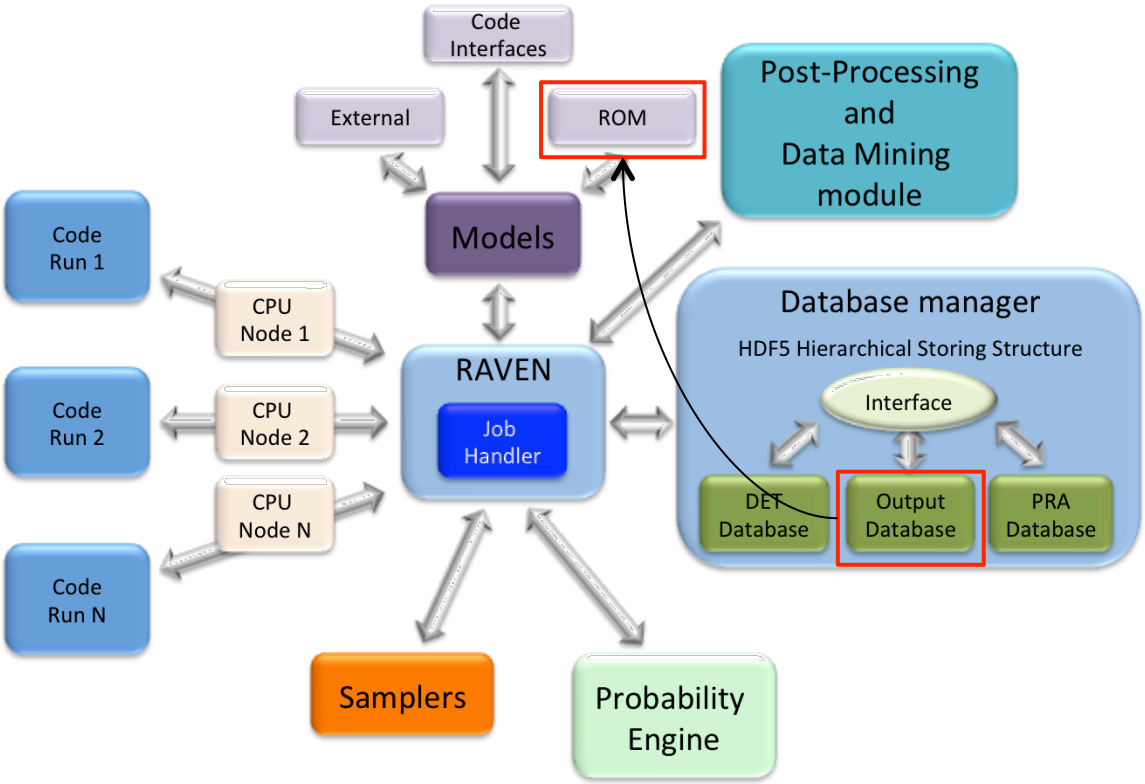
ROM Modeling Within RAVEN

- Create a Database (TimePointSet)



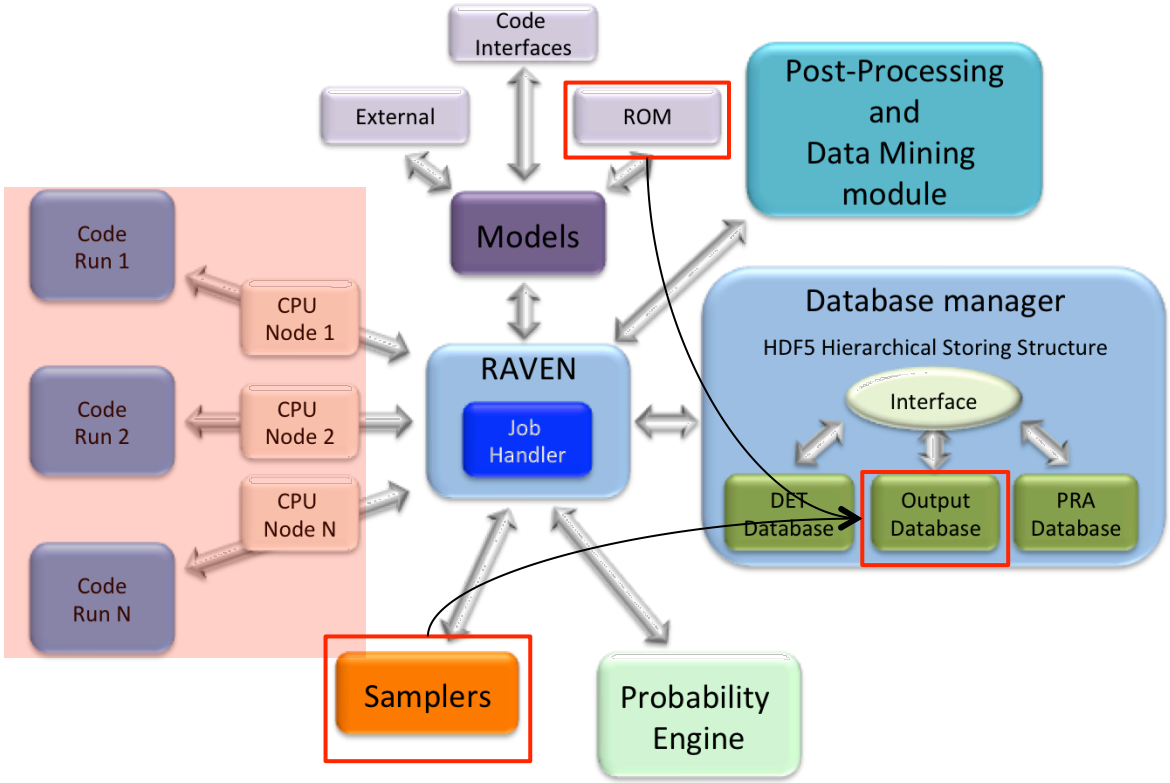
ROM Modeling Within RAVEN

- Create and train a ROM from a Database



ROM Modeling Within RAVEN

- Perform statistical analysis using the ROM



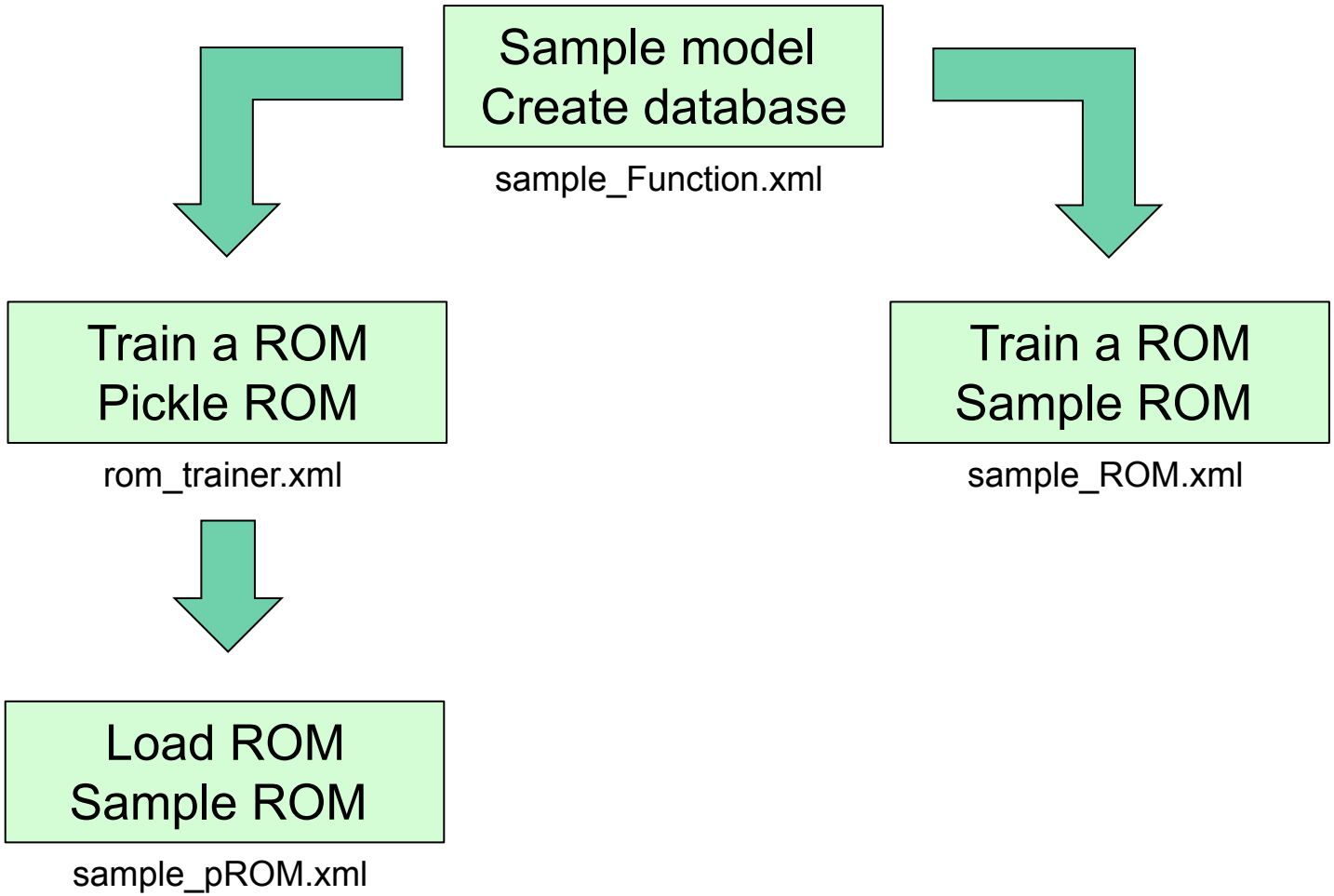
ROM Pickle

- Compression/serialization scheme
- Pickled object contains all the information necessary to reconstruct the object in another python script
- Pickled object can be saved as a file
- RAVEN Scikit-Learn ROMs can be pickled

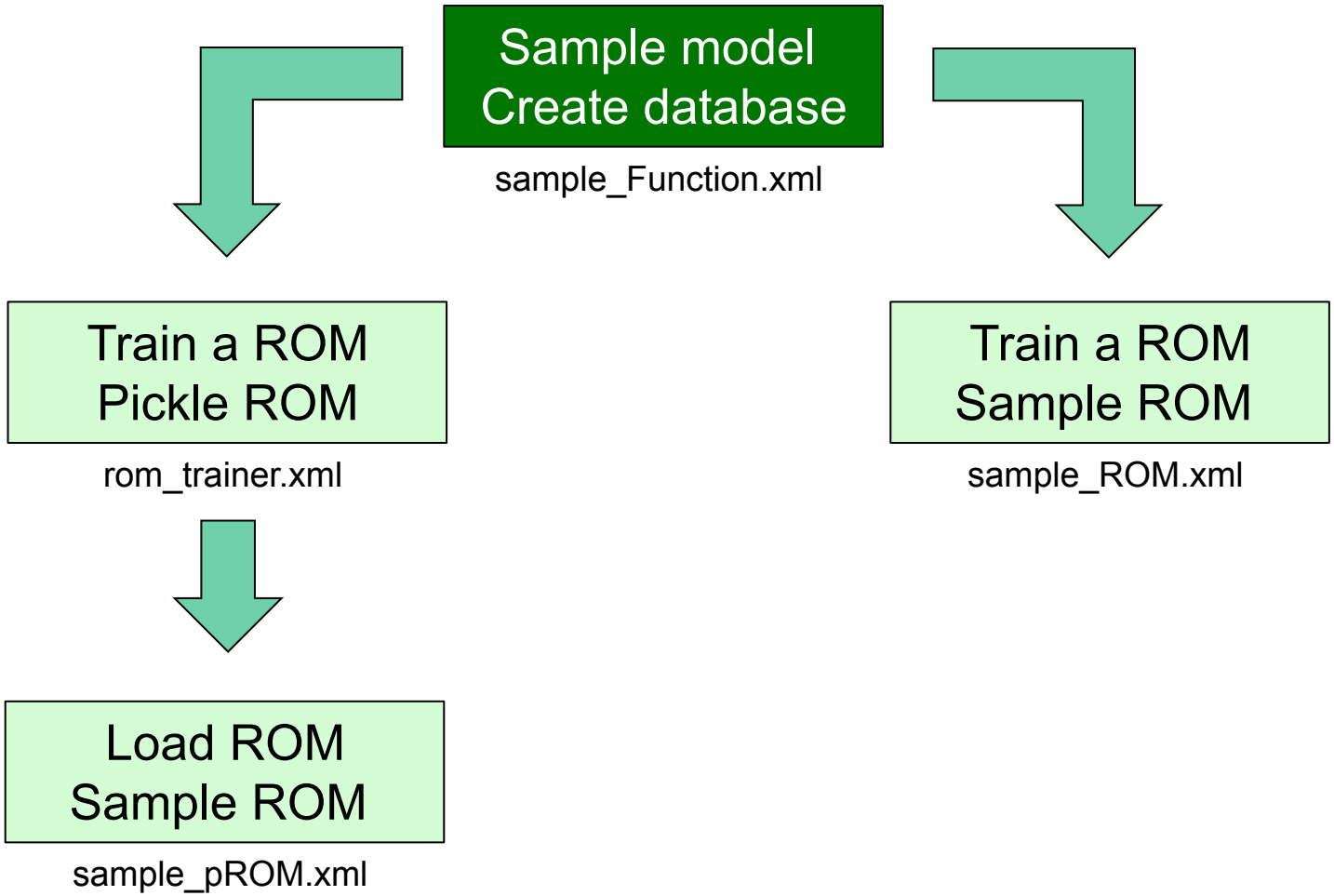
- Applications:
  - Perform statistical analysis on a ROM after they have been generated and/or on a different machine
  - Use pickled ROMs on separate python script (external model for RAVEN)
  - Stochastic analysis for different distributions

RAVEN Examples

Workflow


Sample model
Create database
sample_Function.xml
Train a ROM
Pickle ROM
rom_trainer.xml
Train a ROM
Sample ROM
sample_ROM.xml
Load ROM
Sample ROM
sample_pROM.xml

Workflow


Sample model
Create database
sample_Function.xml
Train a ROM
Pickle ROM
rom_trainer.xml
Load ROM
Sample ROM
sample_pROM.xml
Train a ROM
Sample ROM
sample_ROM.xml

Sample a Model and Create a Database

Distributions	Models	Samplers	Databases	DataObjects	Steps

```
<Distributions>
    <Normal name='normal_trunc'>
        <mean>0.5</mean>
        <sigma>0.1</sigma>
        <lowerBound>0.0</lowerBound>
        <upperBound>1.0</upperBound>
    </Normal>
    <Normal name='normal'>
        <mean>2.0</mean>
        <sigma>0.2</sigma>
    </Normal>
    <Uniform name='uniform'>
        <upperBound>4.0</upperBound>
        <lowerBound>1.0</lowerBound>
    </Uniform>
</Distributions>
```

Truncation parameters

Input file name: sample_Function.xml

Sample a Model and Create a Database

Distributions	Models	Samplers	Databases	DataObjects	Steps

```
<Models>
    <ExternalModel name='PythonModule' subType='' ModuleToLoad='workshop_model'>
       <variable>x1</variable>
       <variable>x2</variable>
       <variable>x3</variable>
       <variable>y1</variable>
       <variable>y2</variable>
       <variable>y3</variable>
       <variable>y4</variable>
       <variable>y5</variable>
    </ExternalModel>
</Models>
```

Input variables

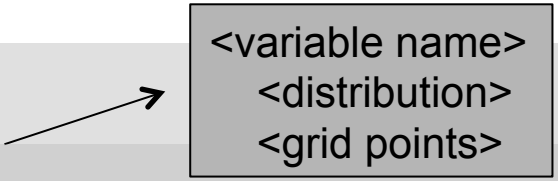
Output variables

File name: workshop_model.py

Input file name: sample_Function.xml

Sample a Model and Create a Database

Distributions	Models	Samplers	Databases	DataObjects	Steps




```
<Samplers>
  <Grid name='Grid_function'>
    <variable name='x1' >
      <distribution>normal_trunc</distribution>
      <grid type='value' lowerBound='0.0' construction='equal' steps='5'>0.2</grid>
    </variable>
    <variable name='x2' >
      <distribution>normal</distribution>
      <grid type='value' lowerBound='1.5' construction='equal' steps='5'>0.2</grid>
    </variable>
    <variable name='x3' >
      <distribution>uniform</distribution>
      <grid type='value' lowerBound='1.0' construction='equal' steps='5'>0.6</grid>
    </variable>
  </Grid>
</Samplers>
```

Input file name: sample_Function.xml

Sample a Model and Create a Database

Distributions	Models	Samplers	Databases	DataObjects	Steps

```
<Databases>
  <HDF5 name='out_db'/>
</Databases>

<DataObjects>
    <TimePointSet name='Data1'>
        <Input>x1,x2,x3</Input>
        <Output>OutputPlaceHolder</Output>
    </TimePointSet>
    <TimePointSet name='inputPlaceHolder'>
        <Input>x1,x2,x3</Input>
        <Output>y1,y2,y3,y4,y5</Output>
   </TimePointSet>
</DataObjects>
```

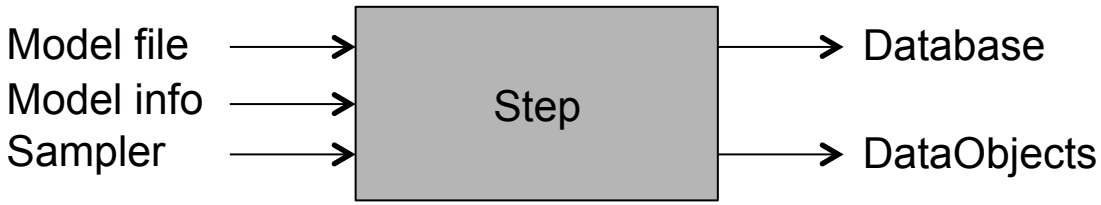
<DataObjects>
<Inputs>
<Output>

Input file name: sample_Function.xml

Sample a Model and Create a Database

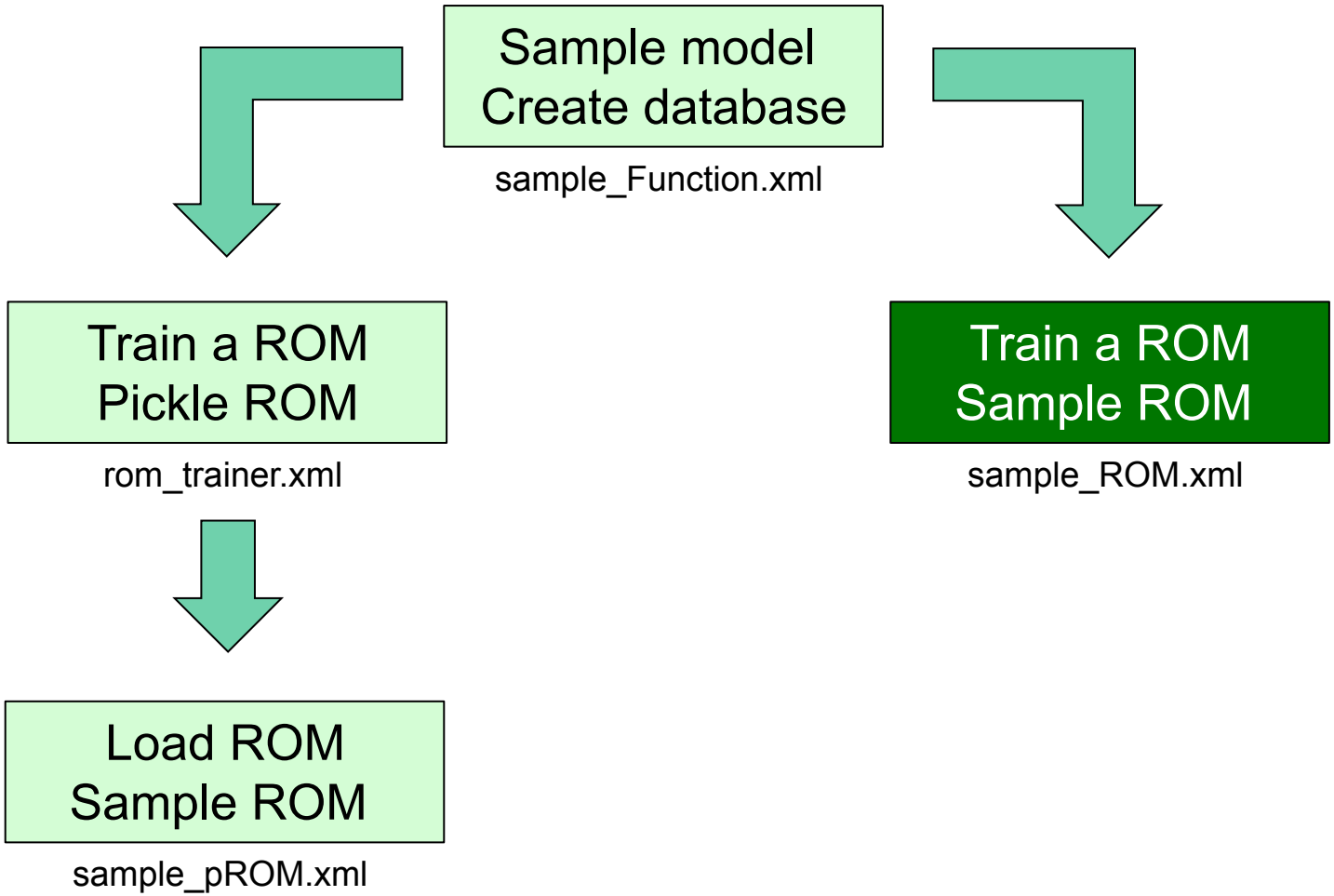
Distributions	Models	Samplers	Databases	DataObjects	Steps

```
<Steps>
  <MultiRun name='FirstMRun'>
    <Input   class='DataObjects' type='TimePoint'    >inputPlaceHolder</Input>
    <Model   class='Models'      type='ExternalModel'>PythonModule</Model>
    <Sampler class='Samplers'    type='Grid'         >Grid_function</Sampler>
    <Output  class='DataObjects' type='TimePointSet' >outGRID</Output>
    <Output  class='Databases'   type='HDF5'         >out_db</Output>
    <Output  class='OutStreamManager' type='Print'   >out_dump</Output>
    <Output  class='OutStreamManager' type='Plot'    >plotResponseFunction</Output>
  </MultiRun>
</Steps>
```



Input file name: sample_Function.xml

Workflow


Sample model
Create database
sample_Function.xml
Train a ROM
Pickle ROM
rom_trainer.xml
Load ROM
Sample ROM
sample_pROM.xml
Train a ROM
Sample ROM
sample_ROM.xml

Train and Sample a ROM

Distributions	Models	Samplers	Databases	DataObjects	Steps

```
<Distributions>
    <Normal name='normal_trunc'>
        <mean>0.5</mean>
        <sigma>0.1</sigma>
        <lowerBound>0.0</lowerBound>
        <upperBound>1.0</upperBound>
    </Normal>
    <Normal name='normal'>
        <mean>2.0</mean>
        <sigma>0.2</sigma>
    </Normal>
    <Uniform name='uniform'>
        <upperBound>4.0</upperBound>
        <lowerBound>1.0</lowerBound>
    </Uniform>
</Distributions>
```

Truncation parameters

Input file name: sample_ROM.xml

Train and Sample a ROM

Distributions	Models	Samplers	Databases	DataObjects	Steps

```
<Models>
    <ROM name='ROM4' subType='NDinvDistWeight'>
      <Features>x1,x2,x3</Features>
      <Target>y4</Target>
      <p>3</p>
    </ROM>
</Models>
```

Multi-dimensional interpolator (CROW)

Input file name: sample_ROM.xml

Train and Sample a ROM

Distributions	Models	Samplers	Databases	DataObjects	Steps

```
<Samplers>
  <Grid name='Grid_ROM'>
    <variable name='x1'>
      <distribution>normal_trunc</distribution>
      <grid type='value' lowerBound='0.0' construction='equal' steps='10'>0.1</grid>
    </variable>
    <variable name='x2'>
      <distribution>normal</distribution>
      <grid type='value' lowerBound='1.5' construction='equal' steps='10'>0.1</grid>
    </variable>
    <variable name='x3'>
      <distribution>uniform</distribution>
      <grid type='value' lowerBound='1.0' construction='equal' steps='10'>0.3</grid>
    </variable>
  </Grid>
</Samplers>
```

Finer grid

Input file name: sample_ROM.xml

Train and Sample a ROM

Distributions	Models	Samplers	Databases	DataObjects	Steps

```
<Databases>
    <HDF5 name='out_db' filename='out_db.h5' directory='path2DB/DBStorage/'/>
</Databases>

<DataObjects>
     <TimePointSet name='outGRID_y4'>
        <Input>x1,x2,x3</Input>
        <Output>y4</Output>
    </TimePointSet>
    <TimePointSet name='outROM_y4'>
        <Input>x1,x2,x3</Input>
        <Output>y4</Output>
    </TimePointSet>
    <TimePointSet name='Data1'>
        <Input>x1,x2,x3</Input>
        <Output>OutputPlaceHolder</Output>
    </TimePointSet>
</DataObjects>
```

Database containing training dataset

Training DataObject

ROM generated DataObject

Input file name: sample_ROM.xml

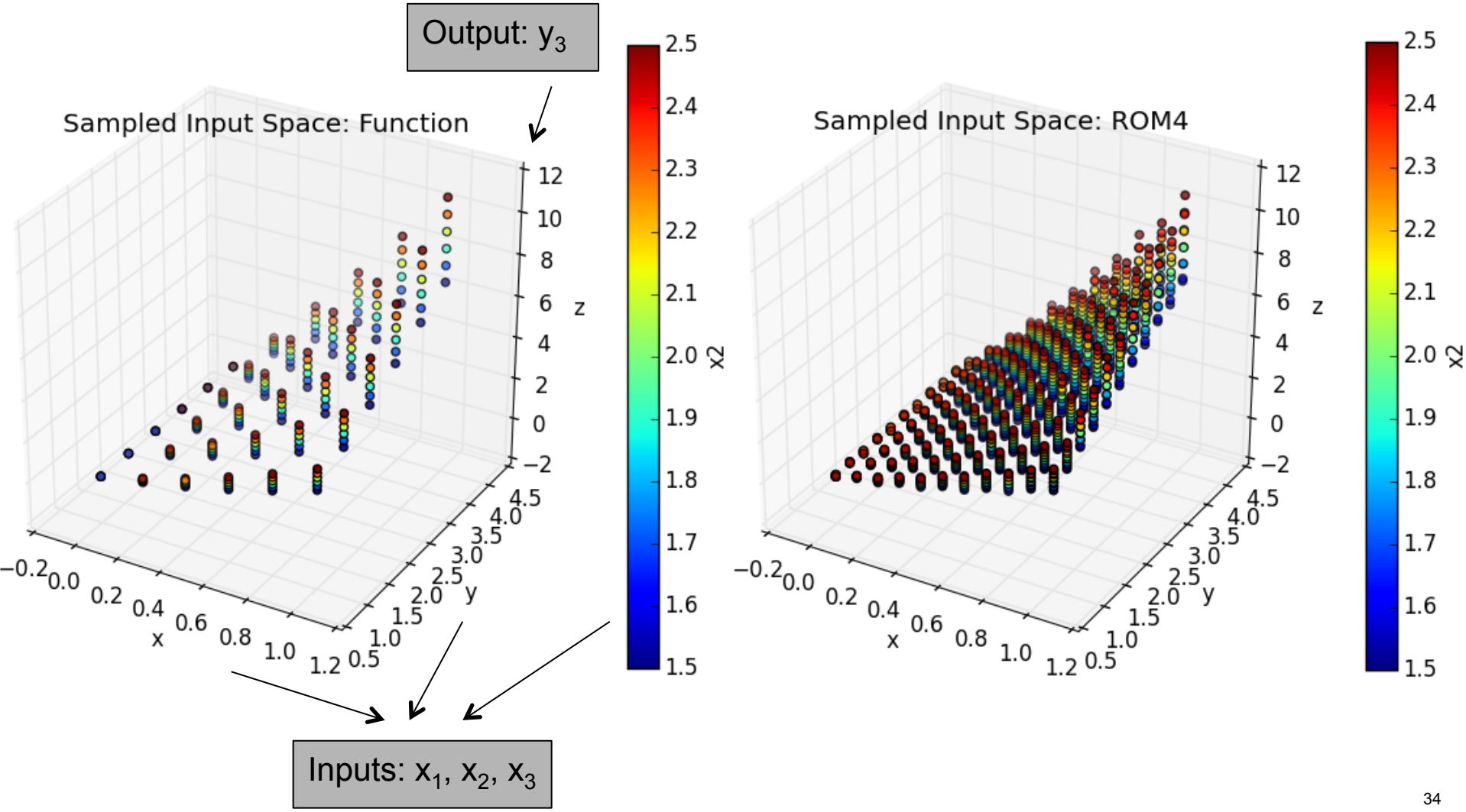
Train and Sample a ROM

Distributions	Models	Samplers	Databases	DataObjects	Steps

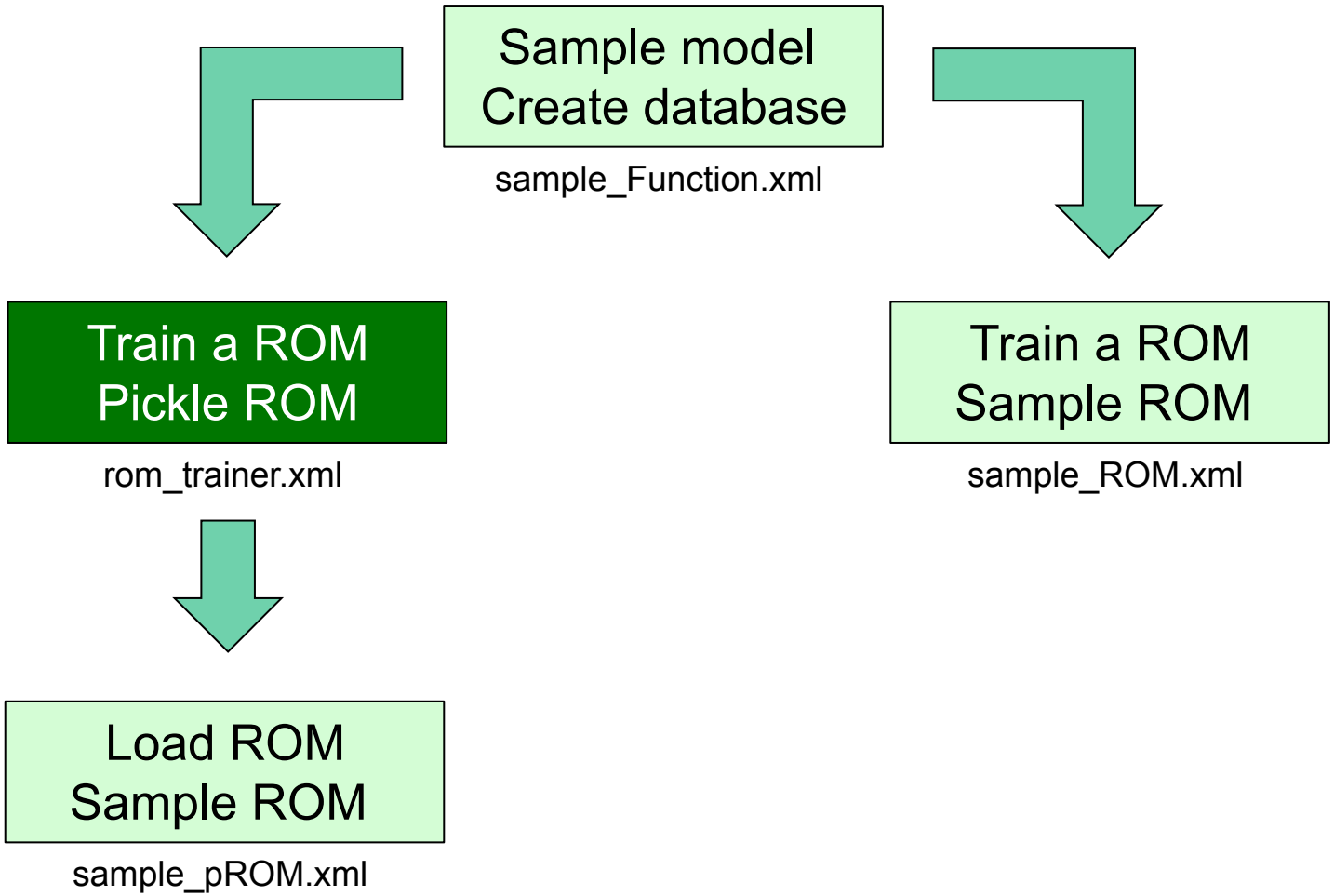
```
<Steps>
  <IOStep name='extract_data4'>
    <Input   class='Databases'   type='HDF5'          >out_db</Input>
    <Output  class='DataObjects' type='TimePointSet' >outGRID_y4</Output>
  </IOStep>
  <RomTrainer name='rom_trainer4'>
    <Input   class='DataObjects' type='TimePointSet' >outGRID_y4</Input>
    <Output  class='Models'      type='ROM'          >ROM4</Output>
  </RomTrainer>
  <MultiRun name='RunRom4'>
    <Input   class='DataObjects' type='TimePointSet' >Data1</Input>
    <Model   class='Models'      type='ROM'          >ROM4</Model>
    <Sampler class='Samplers'    type='Grid'         >Grid_ROM</Sampler>
    <Output  class='DataObjects' type='TimePointSet' >outROM_y4</Output>
</MultiRun>
</Steps>
```

Input file name: sample_ROM.xml

Train and Sample a ROM



Workflow


Sample model
Create database
sample_Function.xml
Train a ROM
Pickle ROM
rom_trainer.xml
Train a ROM
Sample ROM
sample_ROM.xml
Load ROM
Sample ROM
sample_pROM.xml

Train and Pickle a ROM

Models	Databases	DataObjects	Steps

```
<Models>
    <ROM  name='ROM3' subType='SciKitLearn'>
      <Features>x1,x2,x3</Features>
      <Target>y3</Target>
      <SKLtype>linear_model|LinearRegression</SKLtype>
      <fit_intercept>True</fit_intercept>
      <normalize>False</normalize>
    </ROM>
</Models>
```

Inputs / Output

ROM type and parameters

Input file name: rom_trainer.xml

Train and Pickle a ROM

Models	Databases	DataObjects	Steps

```
<Databases>
    <HDF5 name='out_db' filename='out_db.h5' directory='path2DB/DBStorage/'/>
</Databases>


<DataObjects>
    <TimePointSet name='outGRID_y3'>
        <Input>x1,x2,x3</Input>
        <Output>y3</Output>
    </TimePointSet>
</DataObjects>
```

File name and location of the existing database

<DataObjects>
<Multiple Inputs>
<Single Output>

Input file name: rom_trainer.xml

Train and Pickle a ROM

Models	Databases	DataObjects	Steps

```
<Steps>
  <IOStep name='extract_data3'>
    <Input   class='Databases'   type='HDF5'         >out_db</Input>
    <Output  class='DataObjects' type='TimePointSet'>outGRID_y3</Output>
  </IOStep>
  <RomTrainer name='rom_trainer3'>
    <Input   class='DataObjects' type='TimePointSet'>outGRID_y3</Input>
    <Output  class='Models'      type='ROM'          >ROM3</Output>
  </RomTrainer>
  <IOStep name='pkDump3'>
    <Input  class='Models' type='ROM'>ROM3</Input>
    <Output class='Files'  type=''   >ROM3pk</Output>
  </IOStep>
</Steps>
```

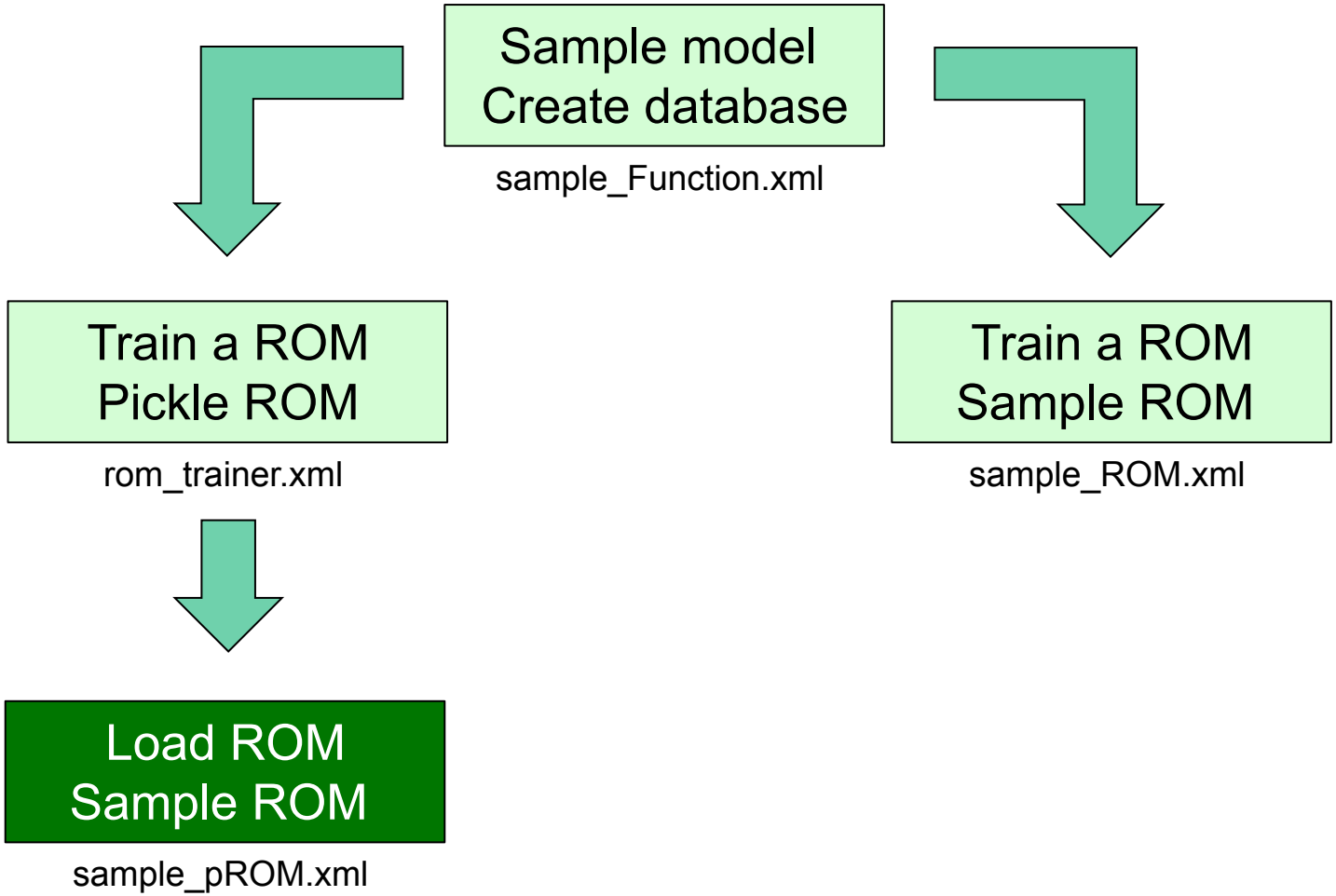
Create a DataObject from the Dababase

Create and train a ROM from the DataObject

Pickle the ROM and save it as a file

Input file name: rom_trainer.xml

Workflow


Sample model
Create database
sample_Function.xml
Train a ROM
Pickle ROM
rom_trainer.xml
Train a ROM
Sample ROM
sample_ROM.xml
Load ROM
Sample ROM
sample_pROM.xml

Load and Sample a Pickled ROM

Distributions	Models	Samplers	DataObjects	Steps

```
<Distributions>
    <Normal name='normal_trunc'>
        <mean>0.5</mean>
        <sigma>0.1</sigma>
        <lowerBound>0.0</lowerBound>
        <upperBound>1.0</upperBound>
    </Normal>
    <Normal name='normal'>
        <mean>2.0</mean>
        <sigma>0.2</sigma>
    </Normal>
    <Uniform name='uniform'>
        <upperBound>4.0</upperBound>
        <lowerBound>1.0</lowerBound>
    </Uniform>
</Distributions>
```

Input file name: sample_pROM.xml

Load and Sample a Pickled ROM

Distributions	Models	Samplers	DataObjects	Steps

```
<Models>
    <ROM  name='ROM3' subType='SciKitLearn'>
      <Features>x1,x2,x3</Features>
      <Target>y3</Target>
      <SKLtype>linear_model|LinearRegression</SKLtype>
      <fit_intercept>True</fit_intercept>
      <normalize>False</normalize>
    </ROM>
</Models>
```

Inputs / Output

ROM type and parameters

Input file name: sample_pROM.xml

Load and Sample a Pickled ROM

Distributions	Models	Samplers	DataObjects	Steps

```
<Samplers>
  <Grid name='Grid_ROM'>
    <variable name='x1'>
      <distribution>normal_trunc</distribution>
      <grid type='value' lowerBound='0.0' construction='equal' steps='10'>0.1</grid>
    </variable>
    <variable name='x2'>
      <distribution>normal</distribution>
      <grid type='value' lowerBound='1.5' construction='equal' steps='10'>0.1</grid>
    </variable>
    <variable name='x3'>
      <distribution>uniform</distribution>
      <grid type='value' lowerBound='1.0' construction='equal' steps='10'>0.3</grid>
    </variable>
  </Grid>
</Samplers>
```

Finer grid

Input file name: sample_pROM.xml

Load and Sample a Pickled ROM

Distributions	Models	Samplers	DataObjects	Steps

```
<DataObjects>
    <TimePointSet name='outPROM_y3'>
        <Input>x1,x2,x3</Input>
        <Output>y3</Output>
    </TimePointSet>
    <TimePointSet name='Data1'>
        <Input>x1,x2,x3</Input>
        <Output>InputPlaceHolder</Output>
    </TimePointSet>
</DataObjects>
```

Input file name: sample_pROM.xml

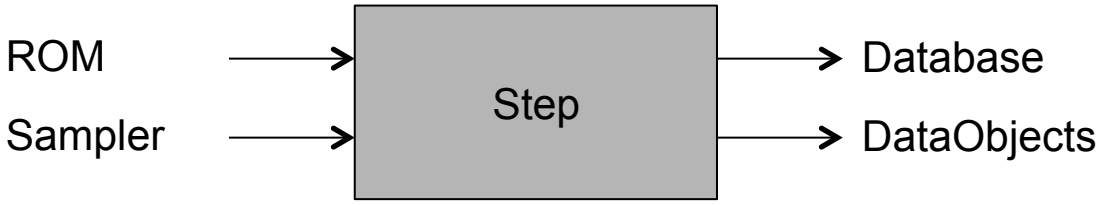
Load and Sample a Pickled ROM

Distributions	Models	Samplers	DataObjects	Steps

```
<Steps>
  <IOStep name='pk3Load'>
    <Input  class='Files'  type=''    >ROM3pk</Input>
    <Output class='Models' type='ROM'>pROM3</Output>
  </IOStep>
  <MultiRun name='RunPROM3'>
    <Input   class='DataObjects' type='TimePointSet'>Data1</Input>
    <Model   class='Models'      type='ROM'          >pROM3</Model>
    <Sampler class='Samplers'    type='Grid'         >Grid_ROM</Sampler>
    <Output  class='DataObjects' type='TimePointSet'>outPROM_y3</Output>
    <Output  class='Databases'   type='HDF5'         >out_ROM3_db</Output>
  </MultiRun>
</Steps>
```

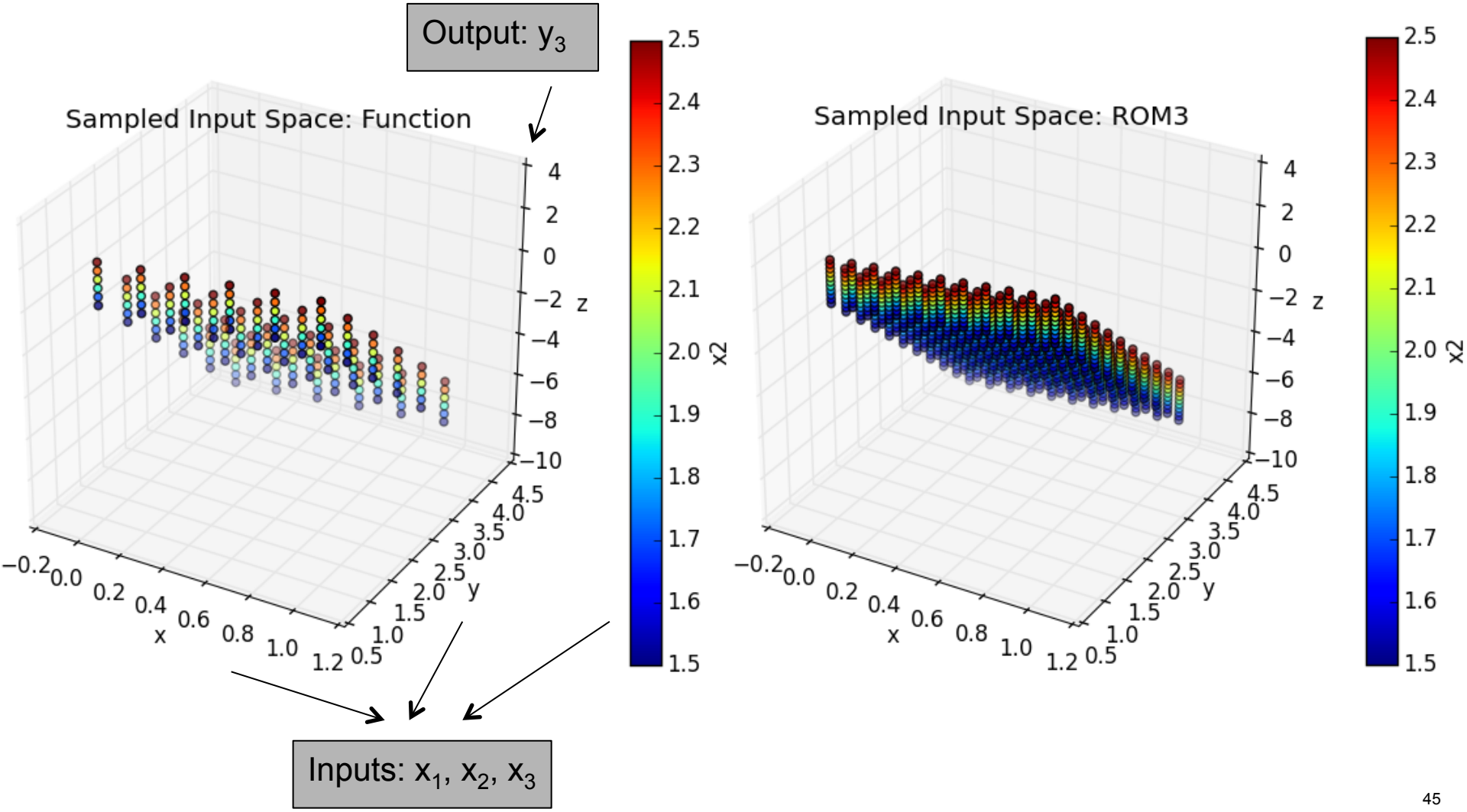
Load the pickled ROM

Sample the pickled ROM



Input file name: sample_pROM.xml

Load and Sample a Pickled ROM



Outline

- Brief introduction on ROMs
- Application examples of ROMs
- ROMs and RAVEN
  - Available ROMs
  - RAVEN ROM workflow
- RAVEN examples
  - Create ROMs
  - Perform sampling of ROMs

Backup slides

Generalized Polynomial Chaos

- Effectiveness depends on:
  - Regularity of quantity of interest $u(Y)$
  - Polynomial expansion order L
  - Polynomial combination indices $\Lambda(L)$
  - Sparse Grid quadrature types (Gauss, Clenshaw)
  - Number of uncertain inputs $N = |Y|$

- Improvements:
  - Use less polynomials
  - Sparse Grid Quadrature