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Test Cases for the Mass-Spring-Damper System

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**Part of the Code Documentation for
Neural Networks for Reduced Order Modeling (ROMNet)**



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A Mass-Spring-Damper Test Case



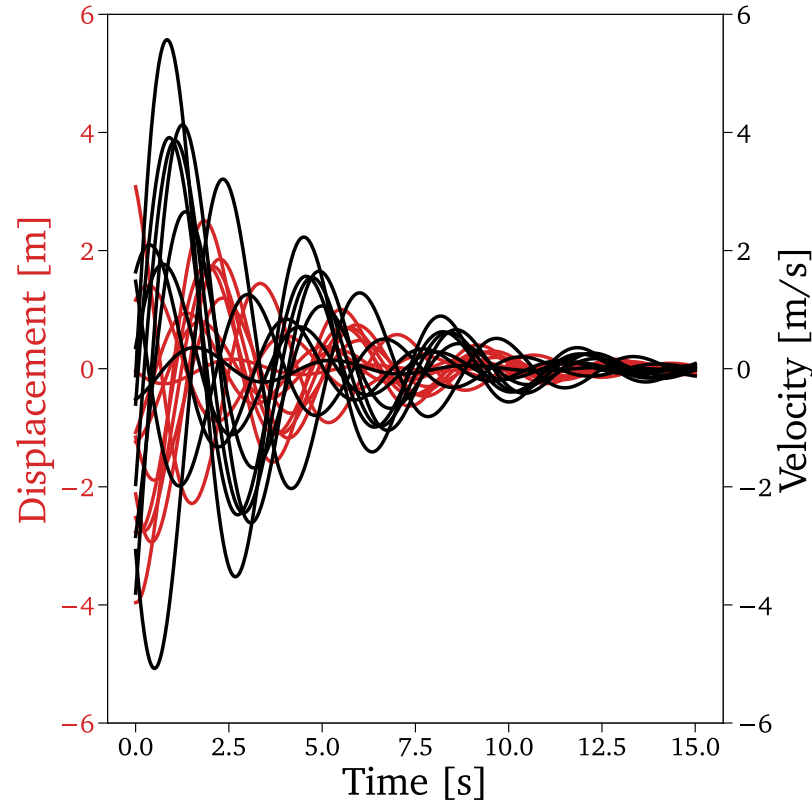
Equations of motion:

$$\begin{cases} m\ddot{x} + c\dot{x} + kx = 0, \\ x(t=0) = x_0, \\ \dot{x}(t=0) = v_0, \end{cases}$$

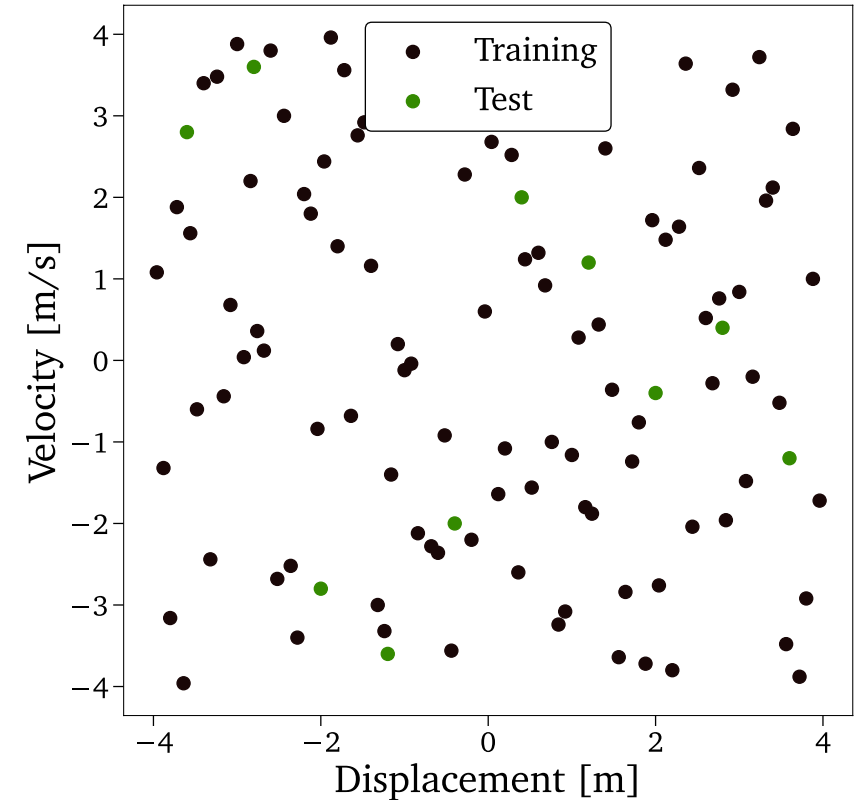
which can be rewritten as:

$$\begin{cases} \begin{bmatrix} \dot{x} \\ \ddot{x} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -\frac{k}{m} & -\frac{c}{m} \end{bmatrix} \begin{bmatrix} x \\ \dot{x} \end{bmatrix} \\ x(t=0) = x_0, \\ \dot{x}(t=0) = v_0. \end{cases}$$

Some training scenarios



Initial conditions



The physical system is implemented in
\$WORKSPACE_PATH/ROMNet/romnet/romnet/pinn/system/massspringdamper.py

The m, c, and k parameters can be found in
\$WORKSPACE_PATH//ROMNet/romnet/database/MassSpringDamper/Params/

A Mass-Spring-Damper Test Case



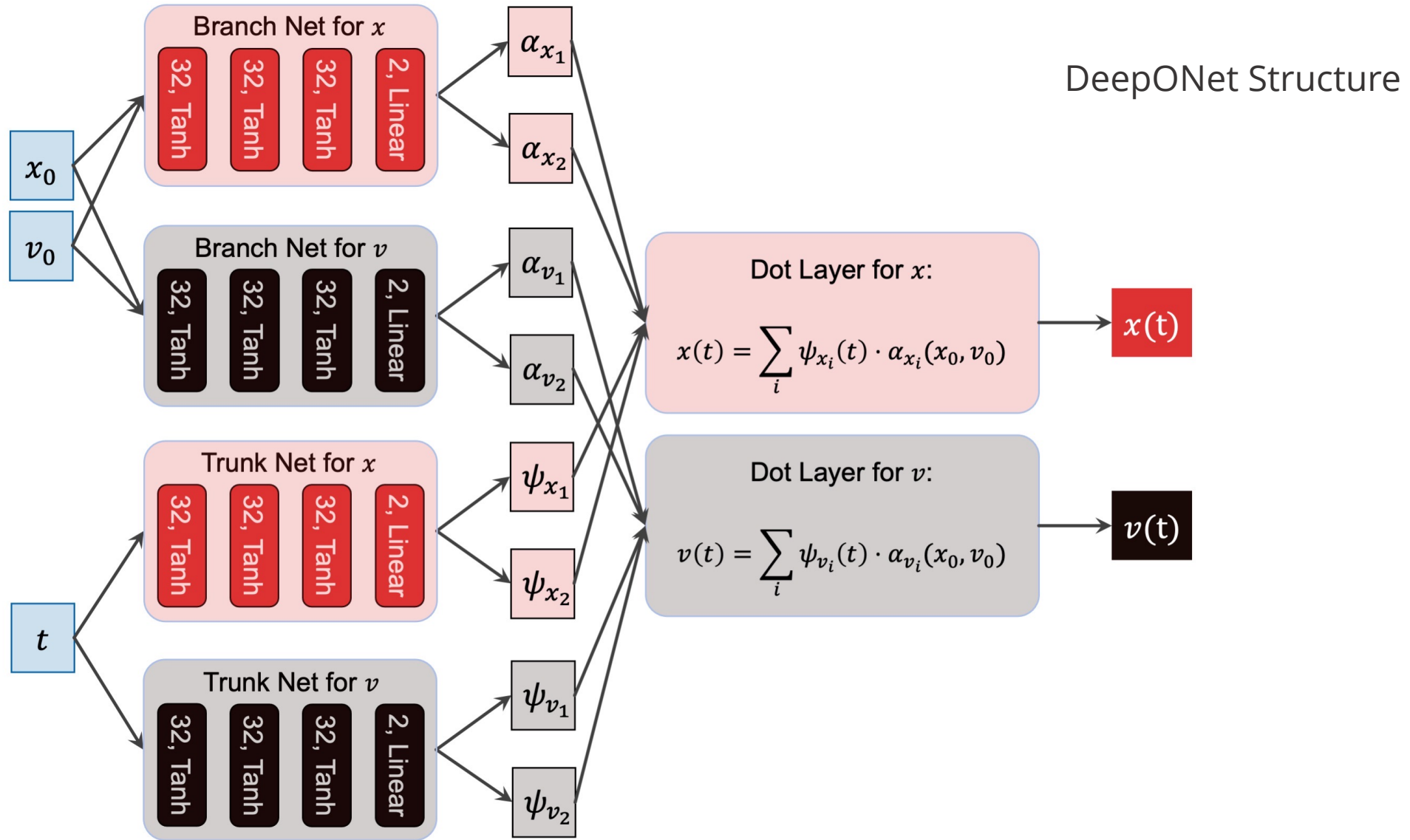
Run Jupyter Notebook
`$WORKSPACE_PATH/ROMNet/romnet/scripts/generating_data/MassSpringDamper/Generate_Data_1.ipynb`
for generating training and test data

A Mass-Spring-Damper Test Case



Test Cases 1 & 2

A Mass-Spring-Damper Test Case

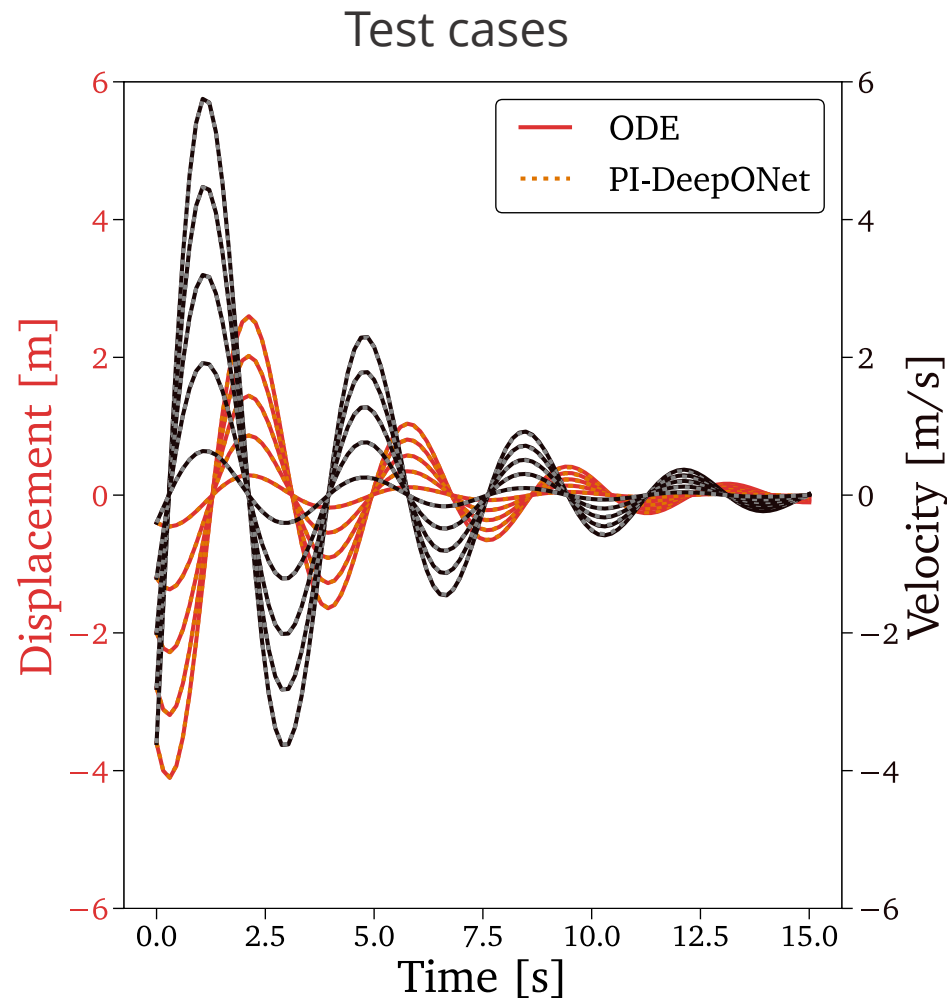


A Mass-Spring-Damper Test Case

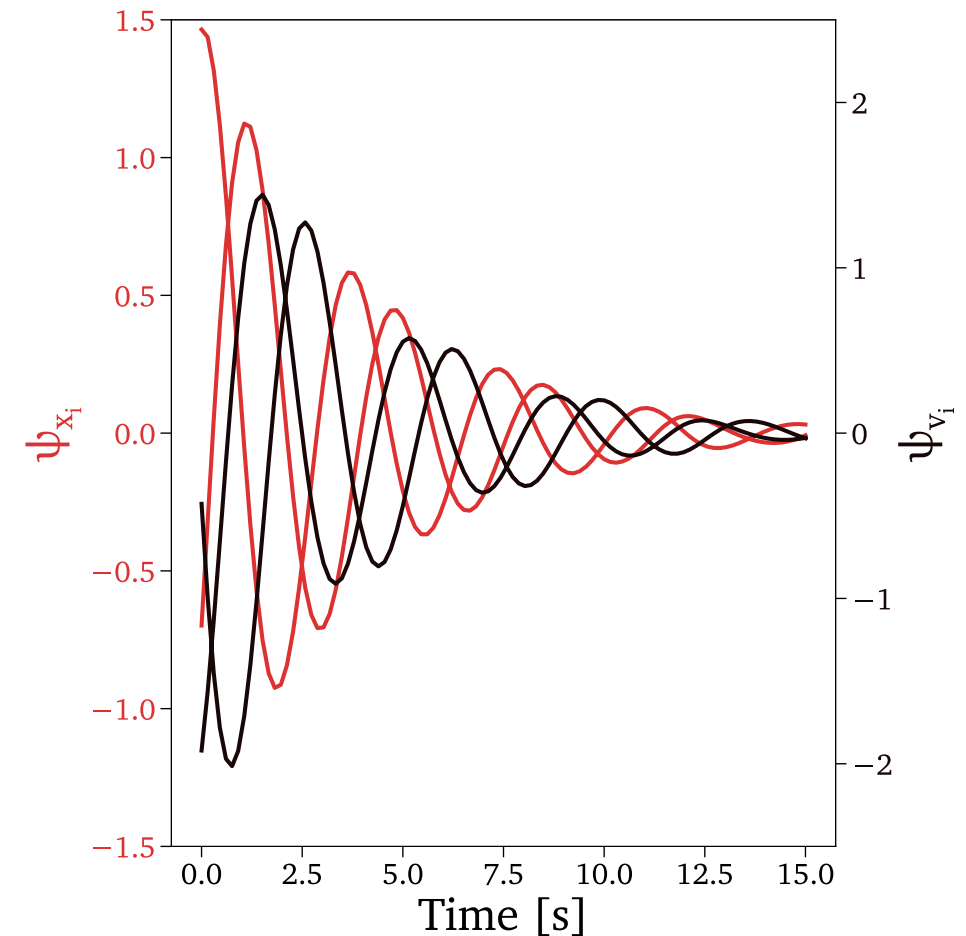


Test Case 1: Fully data-drive training

Test Case 2: Trained with a physics-informed loss



Trunk nets' outputs (~dynamical modes)



A Mass-Spring-Damper Test Case



Test Case 1: Data-driven deep operator network (DeepONet) for predicting position and velocity

- 1.1. Copy `$WORKSPACE_PATH/ROMNet/romnet/input/MassSpringDamper/DeepONet/TestCase1/ROMNet_Input.py`
to `$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py`
- 1.2. In `$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py`, change:
 - 1.2.1. `"self.WORKSPACE_PATH = ..."`
- 1.3. Move to `$WORKSPACE_PATH/ROMNet/romnet/app/`
- 1.4. Run: `"python3 ROMNet.py ../input/"`
- 1.5. Postprocess results via: `$WORKSPACE_PATH/ROMNet/romnet/scripts/postprocessing/MassSpringDamper/DeepONet/Predict_DeepONet.ipynb`

A Mass-Spring-Damper Test Case



Test Case 2: Physics Informed deep operator network (DeepONet) for predicting position and velocity

- 2.1. Copy `$WORKSPACE_PATH/ROMNet/romnet/input/MassSpringDamper/DeepONet/TestCase2/ROMNet_Input.py`
to `$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py`
- 2.2. In `$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py`, change:
 - 2.2.1. `"self.WORKSPACE_PATH = ..."`
- 2.3. Move to `$WORKSPACE_PATH/ROMNet/romnet/app/`
- 2.4. Run: `"python3 ROMNet.py ../input/"`
- 2.5. Postprocess results via: `$WORKSPACE_PATH/ROMNet/romnet/scripts/postprocessing/MassSpringDamper/DeepONet/Predict_DeepONet.ipynb`

In the input file:

self. **surrogate_type** controls the type of surrogate

self.**structure** is a dictionary that controls the structure of the surrogate

Surrogates:

- FNN: Feed-Forward Neural Network
- DeepONet: Deep Operator Network
- Double_DeepONet: Two DeepONets in Series

System of Components:

- FNN
- DeepONet

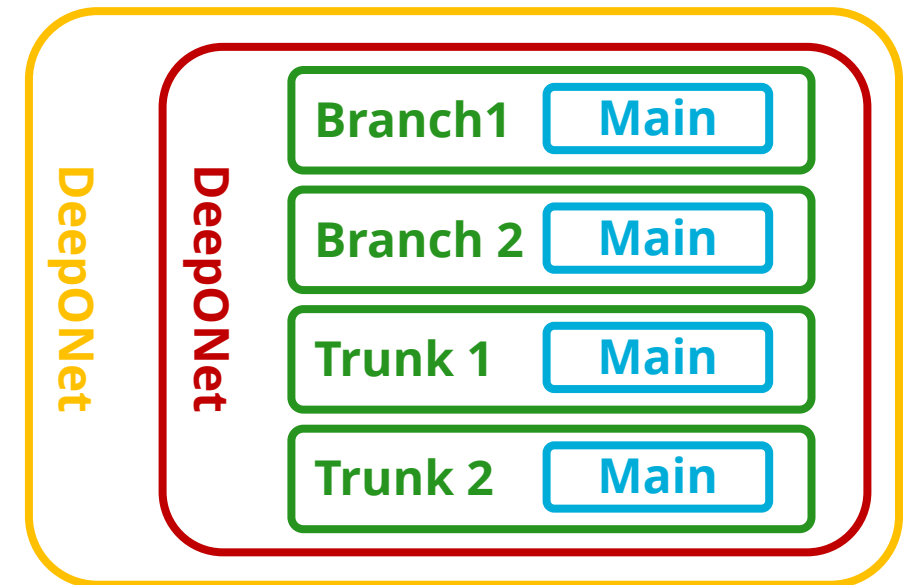
Components:

- FNN
- Branch
- Branch_i
- Trunk
- Trunk_i

Sub-Components:

- Main
- U
- V

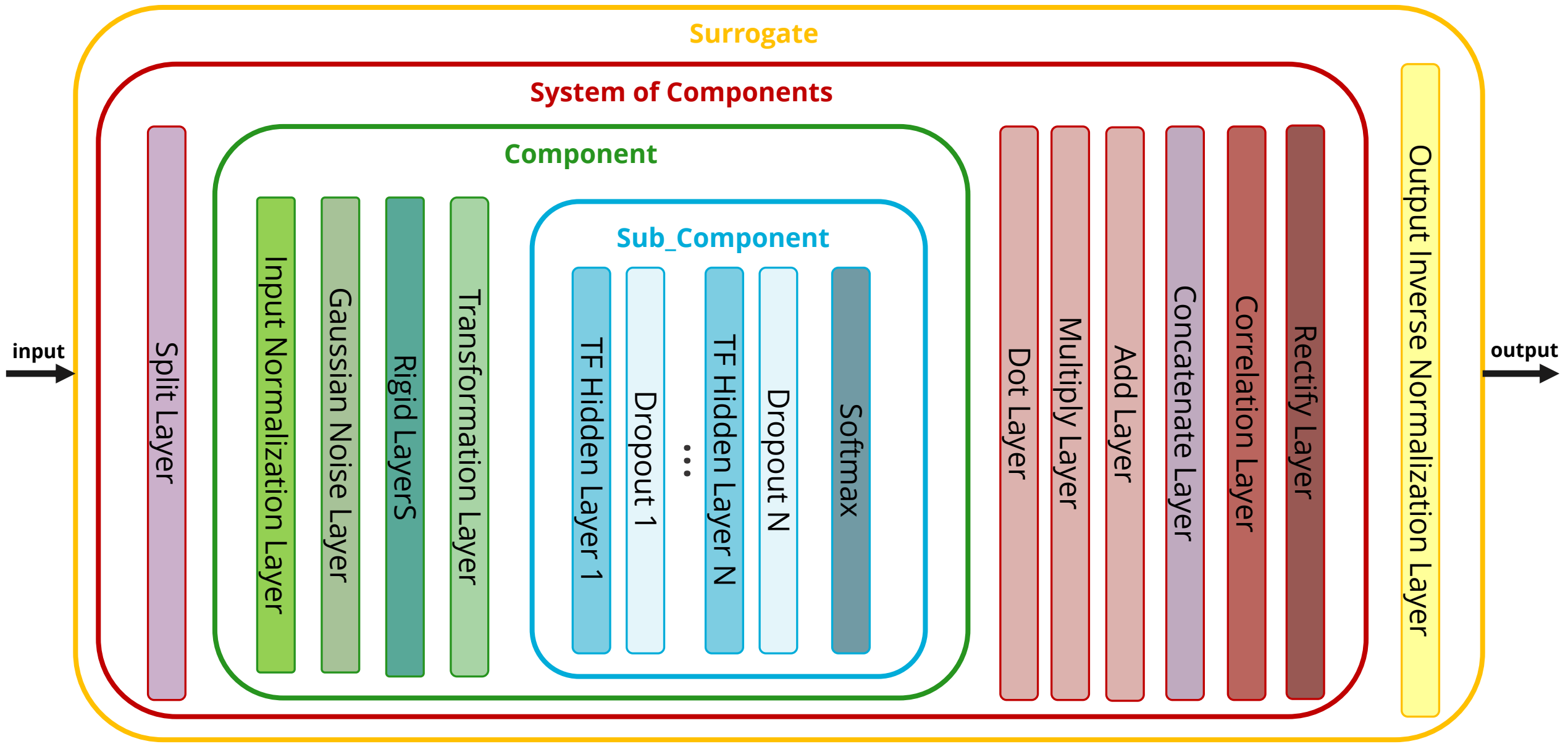
In these test cases:





The related classes can be found in
\$WORKSPACE_PATH/ROMNet/romnet/romnet/nn/

10



The input files for Test Case 1 and 2 differ only for:

self.**n_train** (i.e. Type/No of Data Points)

- 'pts': data point
- 'ics': ODE's initial conditions
- 'res': ODE residual

self. **losses** (i.e., Dictionary Containing Loss Functions for Each Data Type)

self.**loss_weights** (i.e., Dictionary Containing Weights for Each Data Type)



Test Case 3

A Mass-Spring-Damper Test Case



A scenario-aggregated principal component analysis (PCA) analogy

By aggregating the training scenarios for $x_i(t)$ and $v_i(t)$, where i represents the scenario index:

$$X = \begin{bmatrix} | & | & \dots & | & | \\ x_1 & x_2 & \dots & x_{99} & x_{100} \\ | & | & & | & | \end{bmatrix}$$

$$\dim(X) = N_t \times N_s$$

No of time No of
instants scenarios

$$V = \begin{bmatrix} | & | & \dots & | & | \\ v_1 & v_2 & \dots & v_{99} & v_{100} \\ | & | & & | & | \end{bmatrix}$$

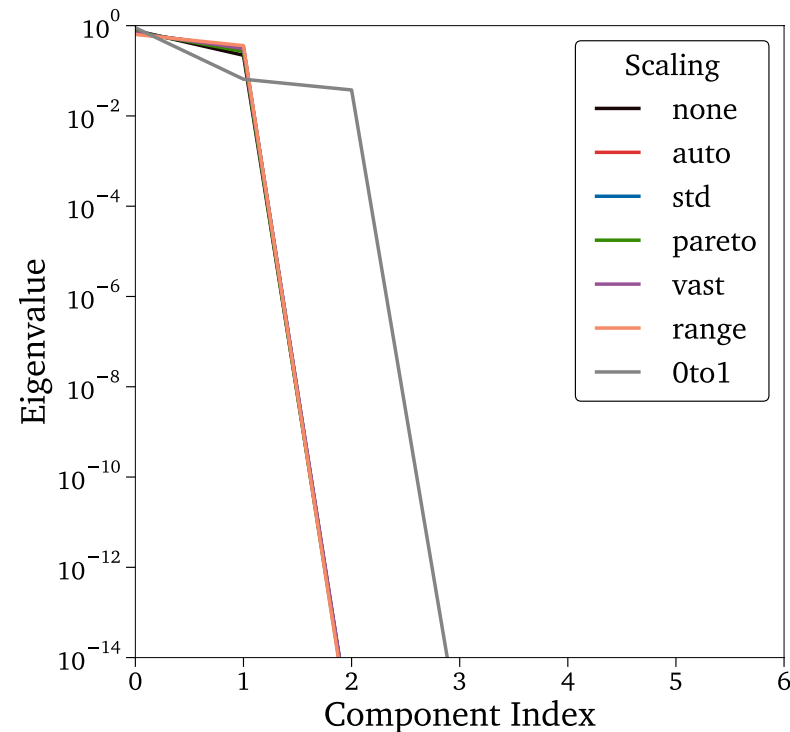
$$\dim(V) = N_t \times N_s$$

A Mass-Spring-Damper Test Case



Eigenvector Decomposition of the Covariance Matrix of X ($\mathbf{R}_X = \frac{\mathbf{X}\mathbf{X}^T}{N_S - 1}$):

Analyzing the eigenvalues:



Eigenvalues of \mathbf{R}_X

$$\Lambda_x = \Psi_x^{-1} \mathbf{R}_x \Psi_x$$

Orthonormal
eigenvectors of \mathbf{R}_X

Two principal components ($N_\psi = 2$) are sufficient for fully characterizing all the 100 scenarios

Note: Equivalent results obtained for the PCA of \mathbf{R}_V

A Mass-Spring-Damper Test Case



Eigenvector Decomposition of the Covariance Matrix of X ($R_x = \frac{XX^T}{N_S - 1}$):

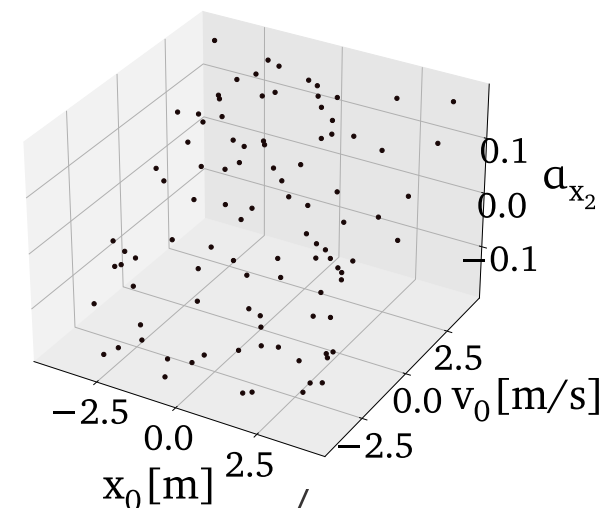
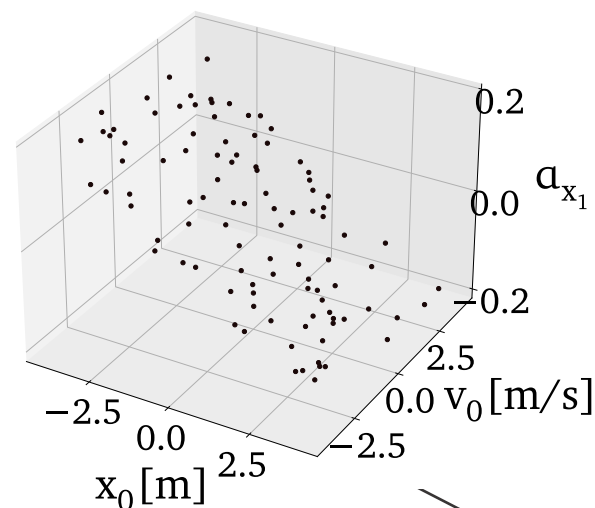
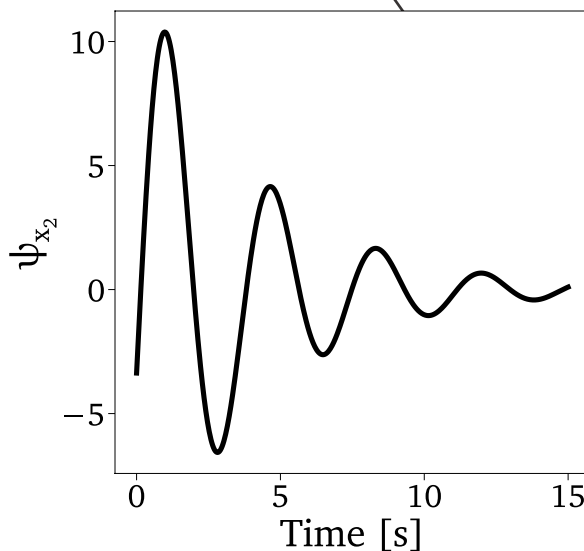
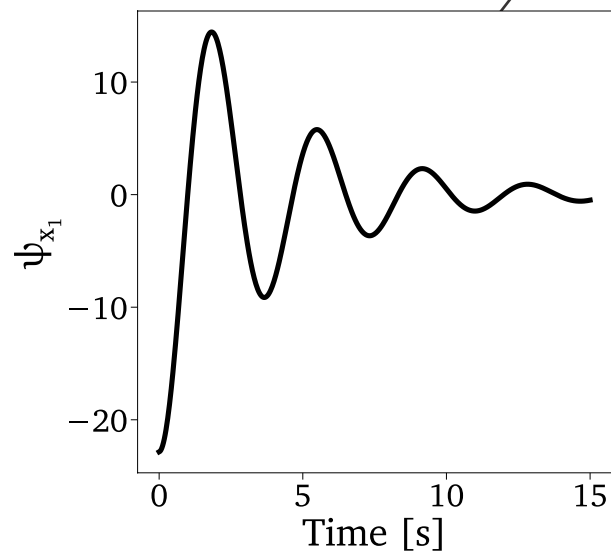
Analyzing the modes and the projection matrix

$$\Psi_x = (X - C_x) \cdot D_x^{-1} A_x =$$

Where:

$$\begin{aligned} \dim(\Psi_x) &= N_t \times N_\psi \\ &= 500 \times 2 \end{aligned}$$

$$\begin{bmatrix} \psi_{x_1} & \psi_{x_2} \end{bmatrix}$$



Where:

$$\begin{aligned} \dim(A_x) &= N_s \times N_\psi \\ &= 100 \times 2 \end{aligned}$$

$$A_x = \begin{bmatrix} \alpha_{x_1} & \alpha_{x_2} \end{bmatrix}$$

A Mass-Spring-Damper Test Case

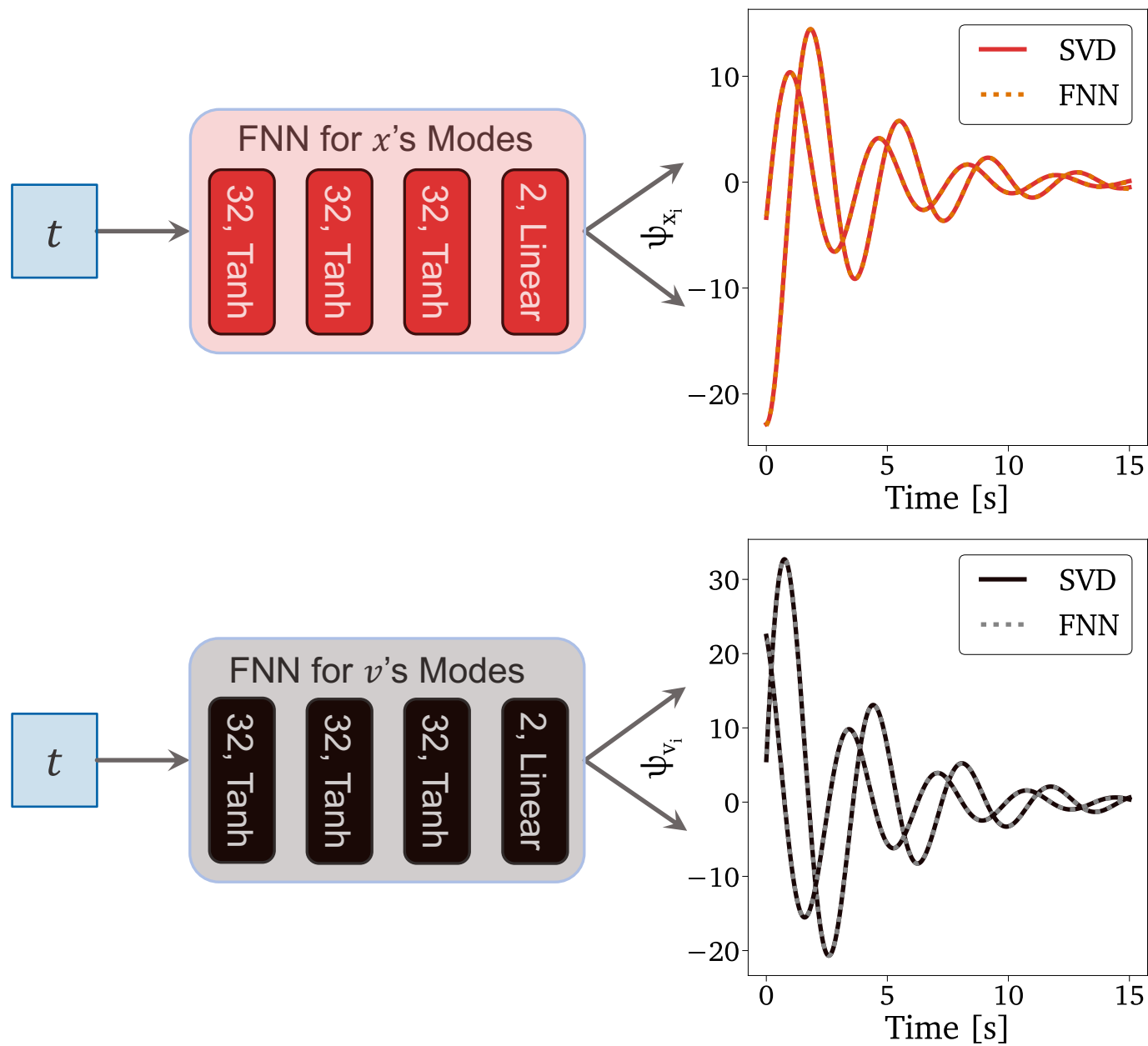


Run Jupyter Notebook

`$WORKSPACE_PATH/ROMNet/romnet/scripts/generating_data/MassSpringDamper/Generate_Data_2.ipynb`
for generating PCA training and test data

Note: The script needs to be run twice, the second time after changing mode_name and i_var

A Mass-Spring-Damper Test Case



Fitted the modes of x and v with two independent feed-forward neural networks

A Mass-Spring-Damper Test Case

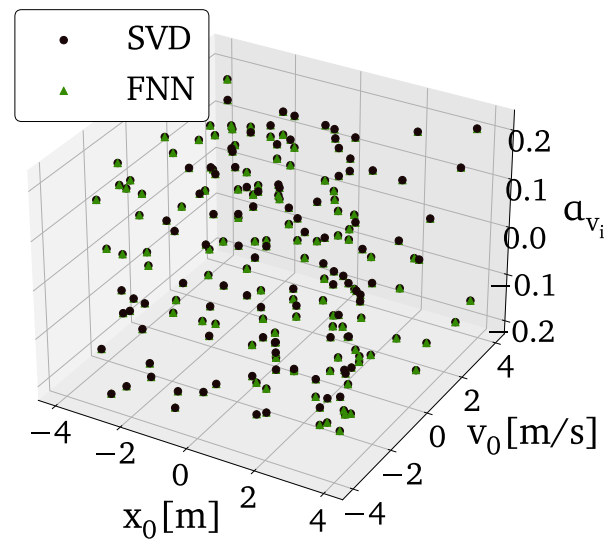
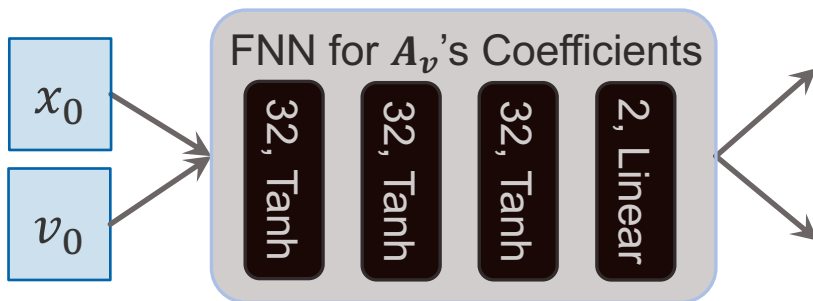
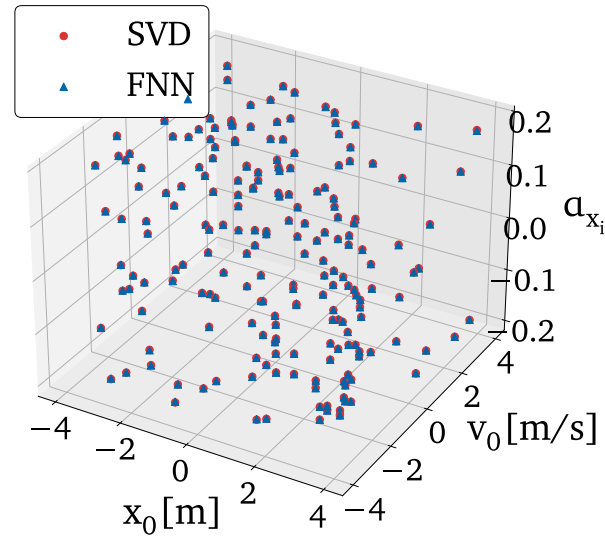
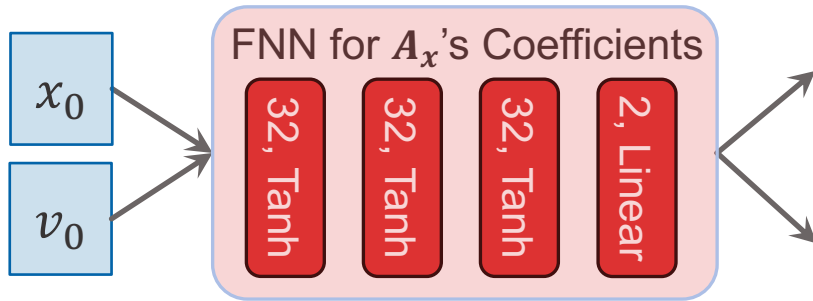


Test Case 3: PCA-based interpretation of DeepONets:

Parts I and II: Train Trunks

- 3.1. Copy `$WORKSPACE_PATH/ROMNet/romnet/input/PCA/MassSpringDamper/FNN/Trunk/TestCase3_Part1/ROMNet_Input.py` to `$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py`
 - 3.2. In `$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py`, change:
 - 3.2.1. `"self.WORKSPACE_PATH = ..."`
 - 3.3. Move to `$WORKSPACE_PATH/ROMNet/romnet/app/`
 - 3.4. Run: `"python3 ROMNet.py ../input/"`
 - 3.5. Postprocess results via: `$WORKSPACE_PATH/ROMNet/romnet/scripts/postprocessing/PCA/MassSpringDamper/FNN/Predict_FNN_Trunk.ipynb`
- REPEAT for the second Trunk (i.e., `$WORKSPACE_PATH/ROMNet/romnet/input/PCA/MassSpringDamper/FNN/Trunk/TestCase3_Part1/ROMNet_Input.py`)

A Mass-Spring-Damper Test Case



Fitted the A_x and A_v components with two independent feed-forward neural networks

A Mass-Spring-Damper Test Case



Test Case 3: PCA-based interpretation of DeepONets:

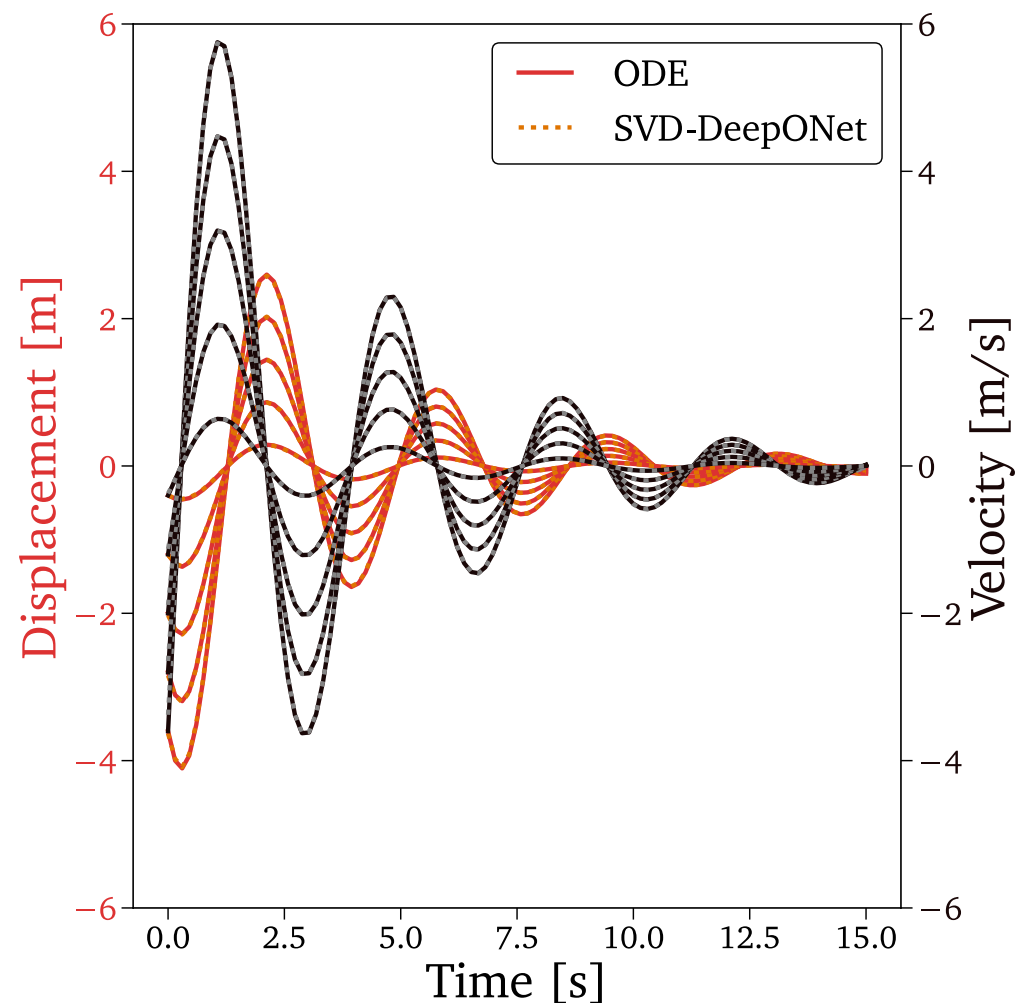
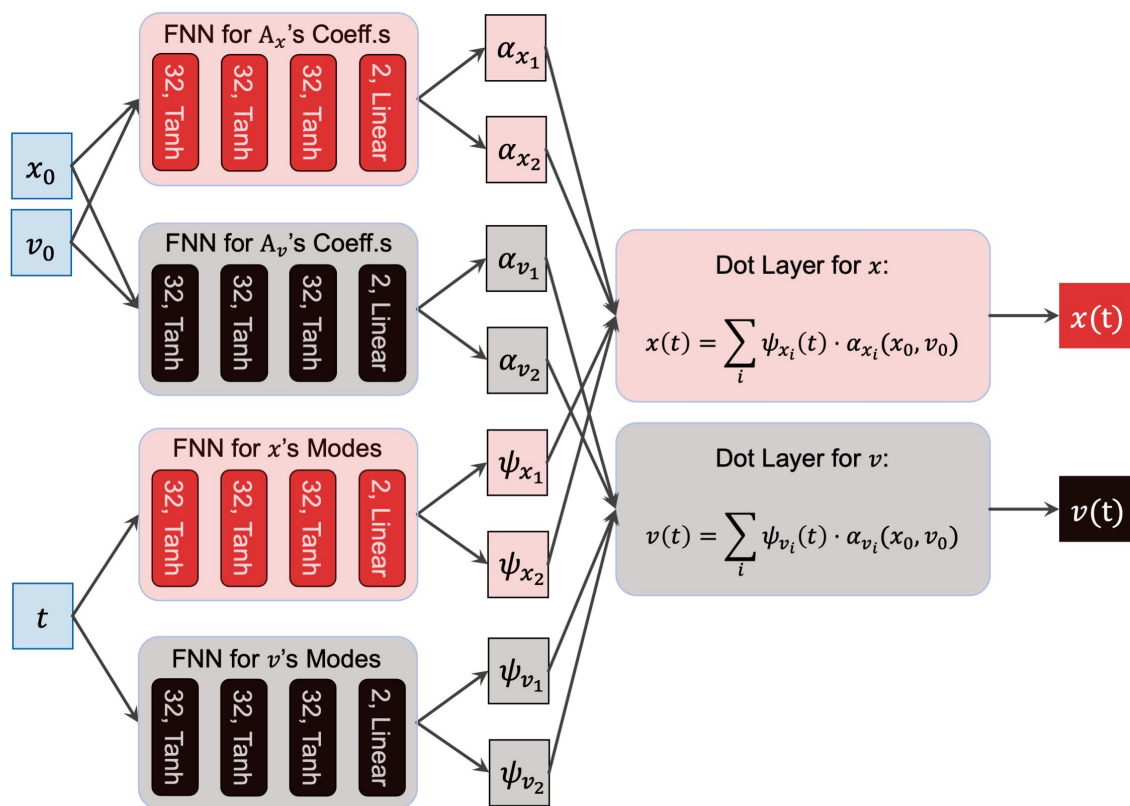
Parts III and IV: Train Branches

- 3.1. Copy `$WORKSPACE_PATH/ROMNet/romnet/input/PCA/MassSpringDamper/FNN/Branch/TestCase3_Part3/ROMNet_Input.py` to `$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py`
 - 3.2. In `$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py`, change:
 - 3.2.1. `"self.WORKSPACE_PATH = ..."`
 - 3.3. Move to `$WORKSPACE_PATH/ROMNet/romnet/app/`
 - 3.4. Run: `"python3 ROMNet.py ../input/"`
 - 3.5. Postprocess results via: `$WORKSPACE_PATH/ROMNet/romnet/scripts/postprocessing/PCA/MassSpringDamper/FNN/Predict_FNN_Branch.ipynb`
- REPEAT for the second Branch (i.e., `$WORKSPACE_PATH/ROMNet/romnet/input/PCA/MassSpringDamper/FNN/Branch/TestCase3_Part4/ROMNet_Input.py`)

A Mass-Spring-Damper Test Case



Generative DeepONet:
 uploaded the parameters of the four FNN's
 as weights and biases of
 the corresponding trunk and branch nets
 and predicted test scenarios (w/o any additional training)



A Mass-Spring-Damper Test Case



Note: If correctly executed, Predict_FNN_Branch.ipynb and Predict_FNN_Trunk.ipynb created the file:
\$WORKSPACE_PATH/ROMNet/Data/MSD_100Cases/Orig/OneByOne/FNN/Final.h5,
which contains the trained parameter values for branches and trunk.

Test Case 3: PCA-based interpretation of DeepONets:

Part V: Generate the DeepONet

- 3.1. Copy \$WORKSPACE_PATH/ROMNet/romnet/input/MassSpringDamper/DeepONet/TestCase3_Part5/ROMNet_Input.py to \$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py
- 3.2. In \$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py, change:
 - 3.2.1. "self.WORKSPACE_PATH = ..."
- 3.3. Move to \$WORKSPACE_PATH/ROMNet/romnet/app/
- 3.4. Run: "python3 ROMNet.py ../input/"
- 3.5. Postprocess results via: \$WORKSPACE_PATH/ROMNet/romnet/scripts/postprocessing/MassSpringDamper/DeepONet/Predict_DeepONet.ipynb

The input files for Test Case 1 differs from the one of Test Case 3 Part 5 for:

self.**path_to_load_fld**: we are now including a path for uploading pre-trained weights

self.**trainable_flg**: we are not training the parameters



Test Case 4

A Mass-Spring-Damper Test Case



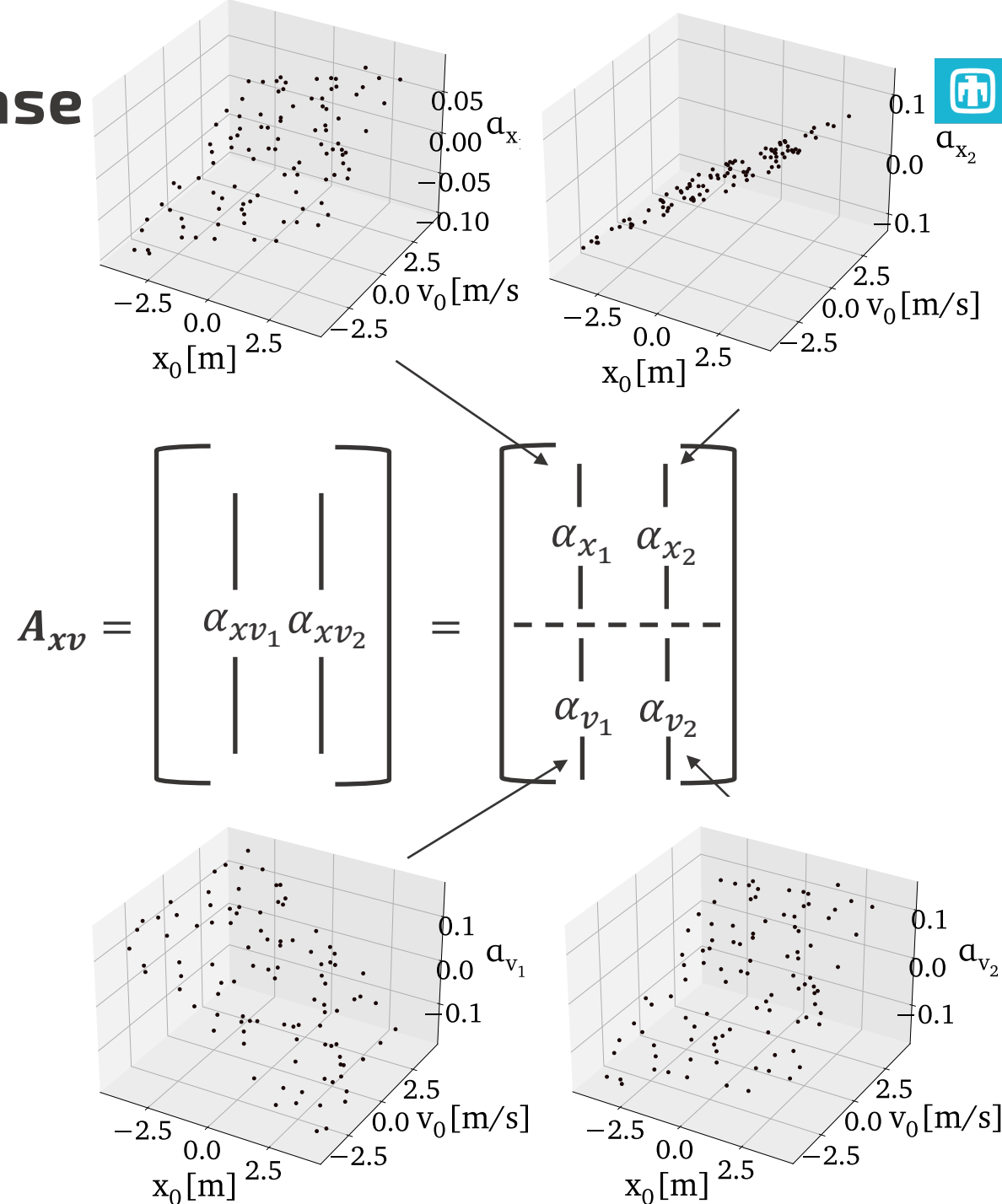
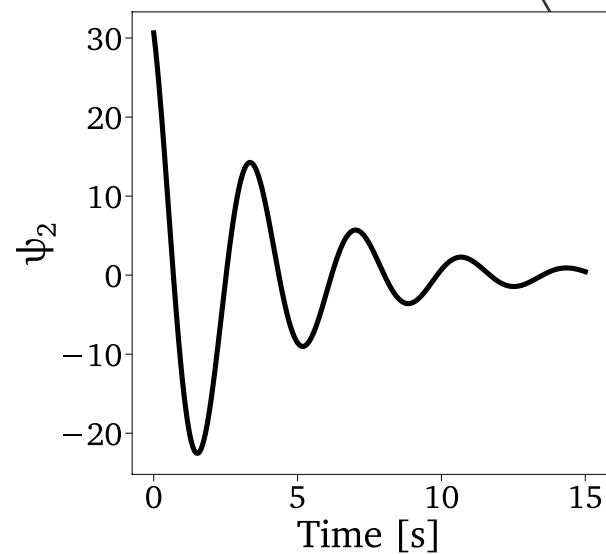
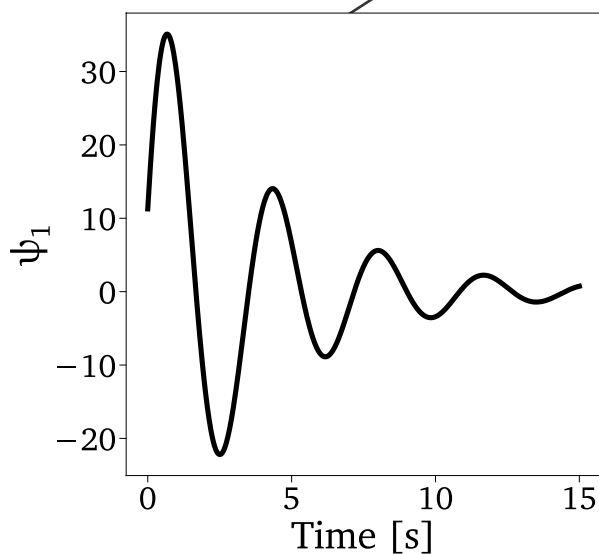
The scenario aggregation can be performed based on one single QoI (as shown so far), resulting in N_y separate trunks, or it can be executed by including all the QoIs simultaneously, resulting in one single trunk.

$$XV = \begin{bmatrix} | & | & & | & | & | & | & & | & | \\ x_1 & x_2 & \dots & x_{99} & x_{100} & v_1 & v_2 & \dots & v_{99} & v_{100} \\ | & | & & | & | & | & | & & | & | \end{bmatrix}$$

$$\dim(XV) = N_t \times 2N_s$$

A Mass-Spring-Damper Test Case

$$\Psi_{xv} = (XV - C_{xv}) \cdot D_{xv}^{-1} A_{xv} = \begin{bmatrix} \psi_1 & \psi_2 \end{bmatrix}$$

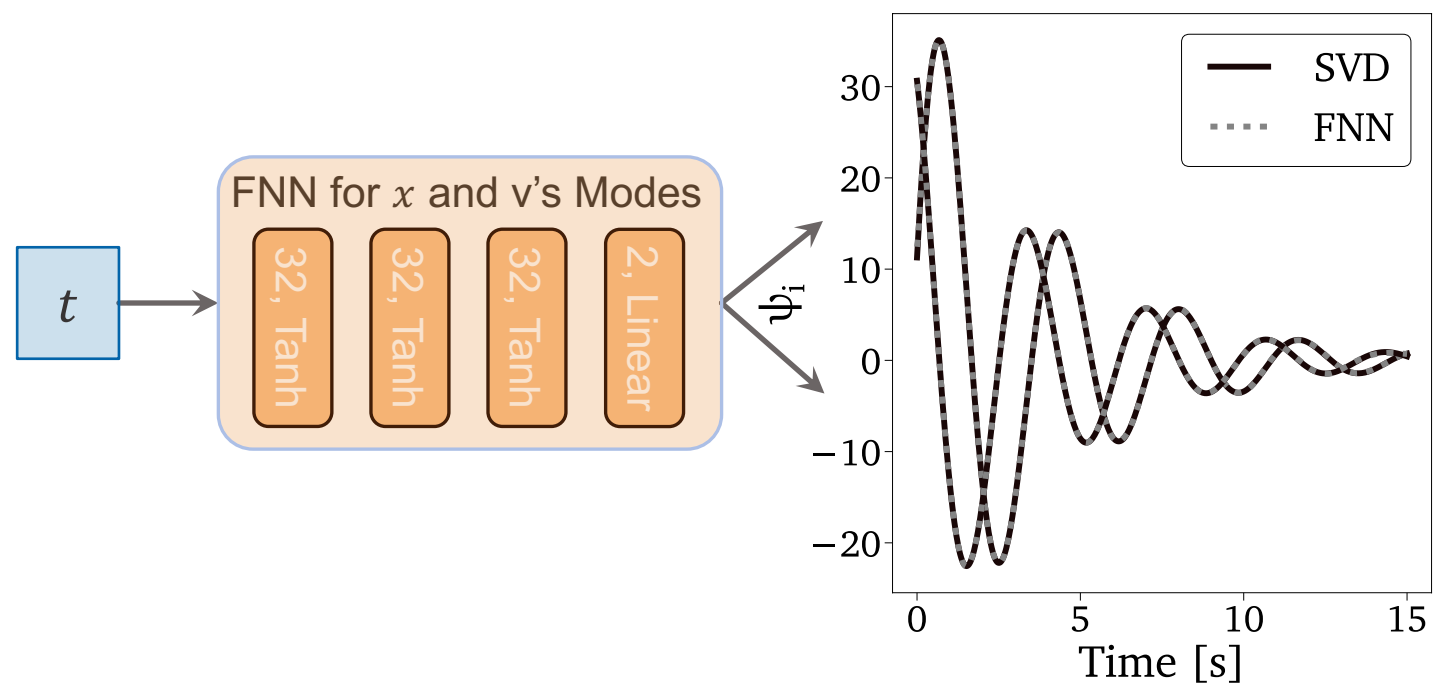


A Mass-Spring-Damper Test Case



Run Jupyter Notebook
\$WORKSPACE_PATH/ROMNet/romnet/scripts/generating_data/MassSpringDamper/Generate_Data_2_All.ipynb
for generating PCA training and test data

A Mass-Spring-Damper Test Case



Fitted the modes of XV
with one
feed-forward neural network

A Mass-Spring-Damper Test Case

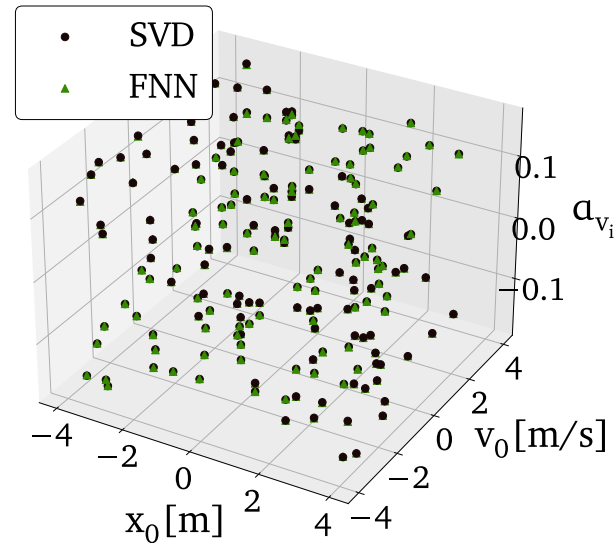
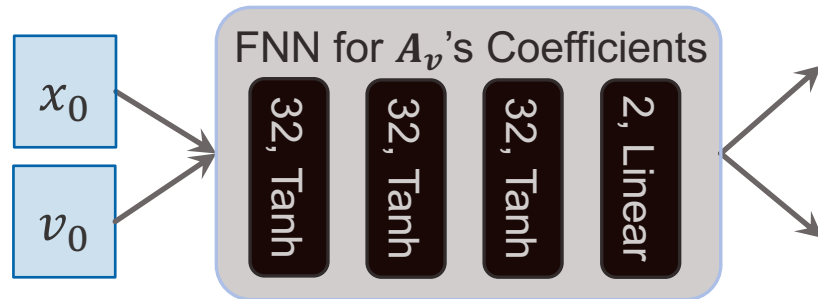
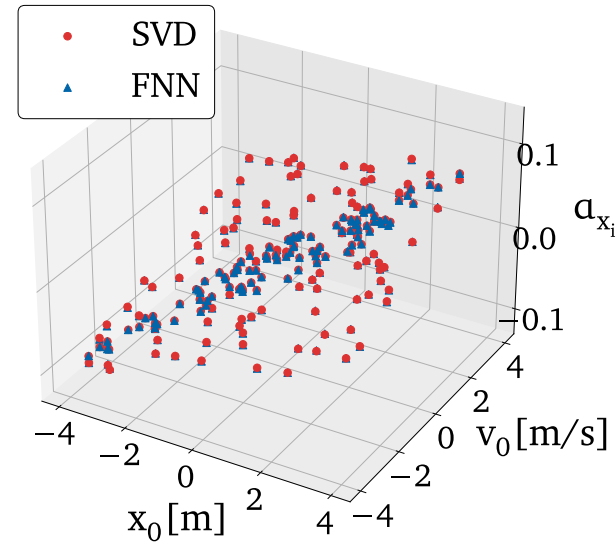
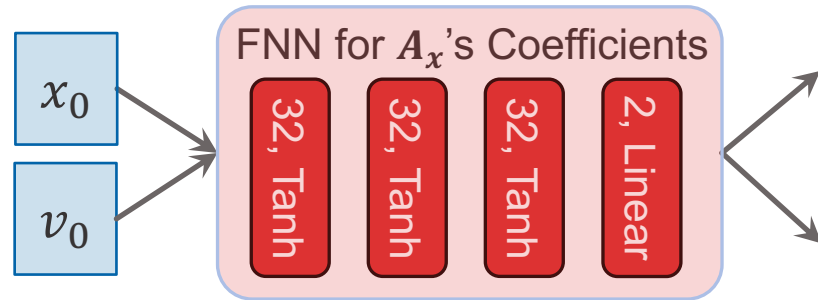


Test Case 4: PCA-based interpretation of DeepONets – Shared Trunk:

Part 1: Train the Trunk

- 4.1. Copy \$WORKSPACE_PATH/ROMNet/romnet/input/PCA/MassSpringDamper/FNN/Trunk/TestCase4_Part1/ROMNet_Input.py to \$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py
- 4.2. In \$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py, change:
 - 4.2.1. "self.WORKSPACE_PATH = ..."
- 4.3. Move to \$WORKSPACE_PATH/ROMNet/romnet/app/
- 4.4. Run: "python3 ROMNet.py ../input/"
- 4.5. Postprocess results via: \$WORKSPACE_PATH/ROMNet/romnet/scripts/postprocessing/PCA/MassSpringDamper/FNN/Predict_FNN_Trunk.ipynb

A Mass-Spring-Damper Test Case



Fitted the A_x and A_v components with two independent feed-forward neural networks

A Mass-Spring-Damper Test Case

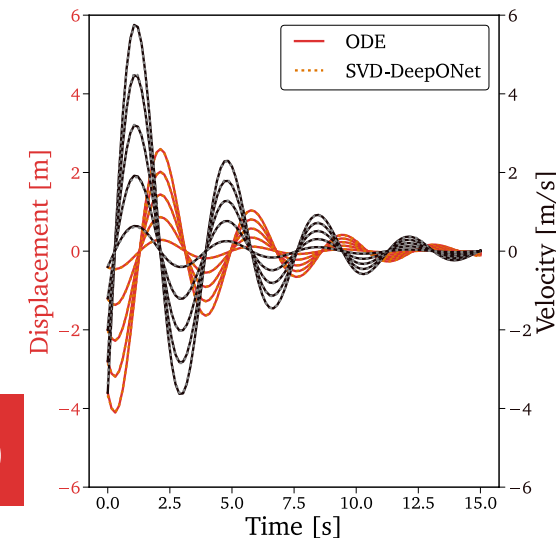
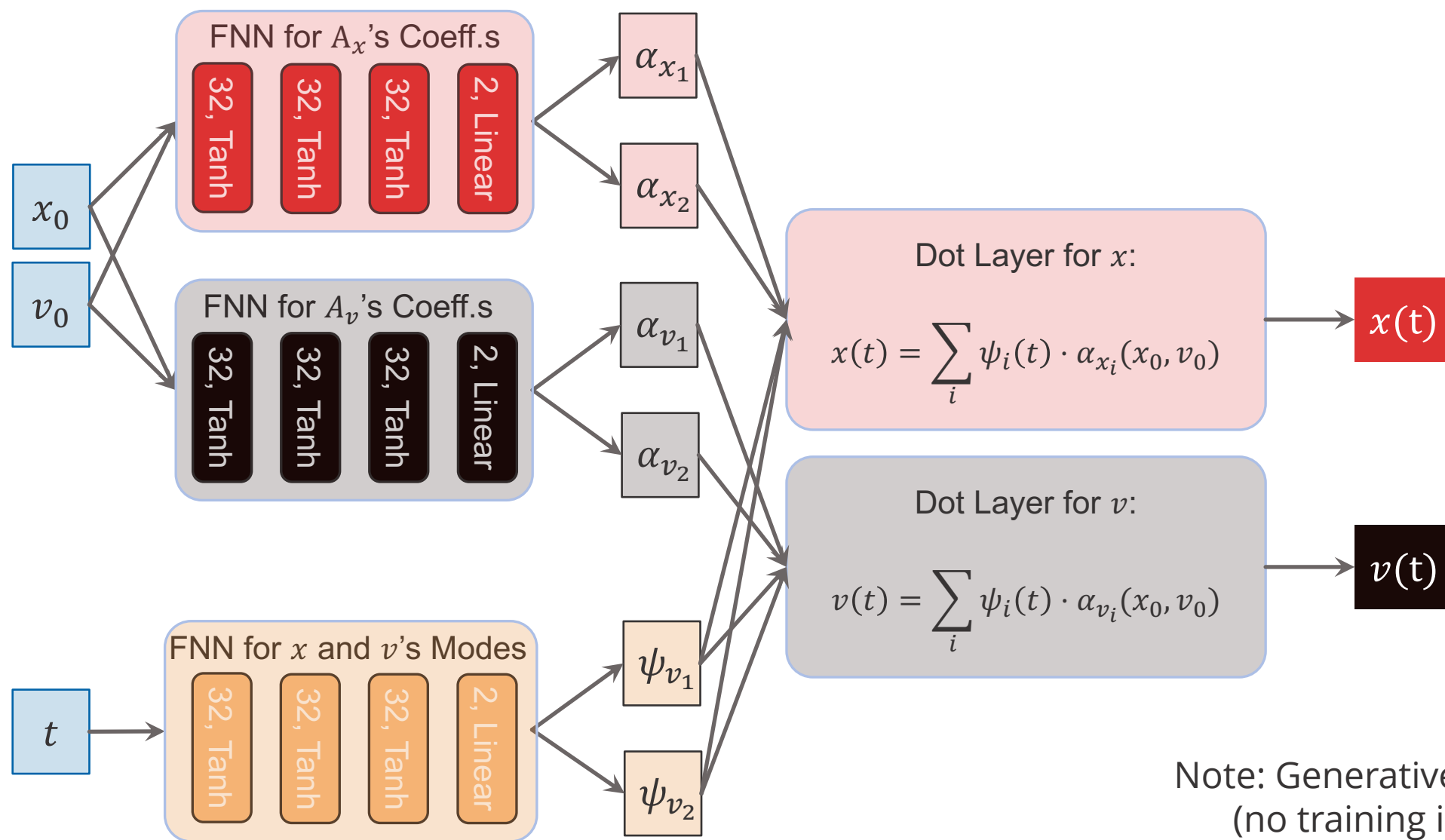


Test Case 4: PCA-based interpretation of DeepONets – Shared Trunk:

Parts II and III: Train Branches

- 4.1. Copy `$WORKSPACE_PATH/ROMNet/romnet/input/PCA/MassSpringDamper/FNN/Branch/TestCase4_Part2/ROMNet_Input.py` to `$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py`
 - 4.2. In `$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py`, change:
 - 4.2.1. `"self.WORKSPACE_PATH = ..."`
 - 4.3. Move to `$WORKSPACE_PATH/ROMNet/romnet/app/`
 - 4.4. Run: `"python3 ROMNet.py ../input/"`
 - 4.5. Postprocess results via: `$WORKSPACE_PATH/ROMNet/romnet/scripts/postprocessing/PCA/MassSpringDamper/FNN/Predict_FNN_Branch.ipynb`
- REPEAT for the second Branch (i.e., `$WORKSPACE_PATH/ROMNet/romnet/input/PCA/MassSpringDamper/FNN/Branch/TestCase4_Part3/ROMNet_Input.py`)

A Mass-Spring-Damper Test Case



Note: Generative DeepONet
(no training involved)

A Mass-Spring-Damper Test Case



Note: If correctly executed, Predict_FNN_Branch.ipynb and Predict_FNN_Trunk.ipynb created the file:
\$WORKSPACE_PATH/ROMNet/Data/MSD_100Cases/Orig/All/FNN/Final.h5,
which contains the trained parameter values for branches and trunk.

Test Case 4: PCA-based interpretation of DeepONets – Shared Trunk:

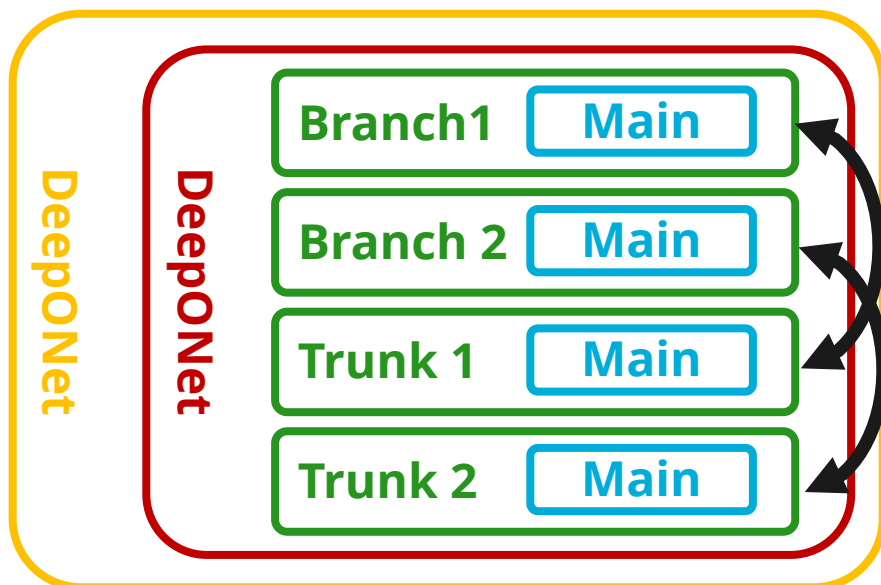
Part IV: Generate the DeepONet

- 4.1. Copy \$WORKSPACE_PATH/ROMNet/romnet/input/MassSpringDamper/DeepONet/TestCase4_Part4/ROMNet_Input.py to \$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py
- 4.2. In \$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py, change:
 - 4.2.1. "self.WORKSPACE_PATH = ..."
- 4.3. Move to \$WORKSPACE_PATH/ROMNet/romnet/app/
- 4.4. Run: "python3 ROMNet.py ../input/"
- 4.5. Postprocess results via: \$WORKSPACE_PATH/ROMNet/romnet/scripts/postprocessing/MassSpringDamper/DeepONet/Predict_DeepONet.ipynb

The input file for Test Case 5 Part 5 differs from the one of Test Case 4 Part 4 for:

`self.branch_to_trunk`: DeepONet Branch-to-Trunk Type of Mapping ('one_to_one'/'multi_to_one')

Test Case 3 Part 5:



Test Case 4 Part 4:

