

Project VAMPnets

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Abstract

- Using numpy, load the provided data from the file ‘5d-folding.npy’. This is a system consisting of a single point moving in a 5-dimensional space, but whose behaviour depends only on its euclidean norm, or distance of the point from the center.
- Build a network that extracts the main slow process(es) in the system, and identify the corresponding timescale value. This requires you to start from a higher number of output nodes, study the result, then go lower until all the timescales are properly estimated
- Add a bottleneck with y nodes, followed by a layer with 10 nodes. Find the minimum value of y that allows you to recover the main timescale correctly. Is the dimensionality of the bottleneck relate to the description of the system?
- Plot the correlation between the distance of your system from the center and the outputs of the bottleneck layer in a scatter plot. (You need to be able to read out the activation of the nodes from a hidden layer)
- Plot the correlation between the outputs of the bottleneck layer and the eigenfunction of the estimated Koopman operator.