ADP_backbone_LSS

May 22, 2025

1 LSS applied to backbone generation of Alanine dipeptide (ADP)

GitHub: https://github.com/andrewlferguson/IMSI_LSS https://github.com/Ferg-Lab/LSS

Paper: @article{sidky2020molecular, title={Molecular latent space simulators}, author={Sidky, Hythem and Chen, Wei and Ferguson, Andrew L}, journal={Chemical Science}, volume={11}, number={35}, pages={9459–9467}, year={2020}, publisher={Royal Society of Chemistry} }

Tutorial: @article{jones2024tutorial, title={Tutorial on Molecular Latent Space Simulators (LSSs): Spatially and temporally continuous data-driven surrogate dynamical models of molecular systems}, author={Jones, Michael S and Shmilovich, Kirill and Ferguson, Andrew L}, journal={Journal of Physical Chemistry A}, volume={128}, pages={10299–10317}, year={2024}, publisher={American Chemical Society}, doi={https://doi.org/10.1021/acs.jpca.4c05389} }

1.1 Allocating GPU accelerator (~1 min)

[1]:
```
import torch
```

[2]:
```
if torch.cuda.is_available():
  print('GPU available')
else:
  print('Please set GPU via Edit -> Notebook Settings.')
```

```
GPU available
```

[3]:
```
device= 'cuda' if torch.cuda.is_available() else 'cpu'
device
```

[3]:
```
'cuda'
```

2 Uploading files (~3 mins)

2.0.1 (i) alanine-dipeptide-0-250ns-nowater.xtc

2.0.2 (ii) alanine-dipeptide-nowater.pdb

N.B. If file upload fails, try using alternate upload means by clicking on file icon in left menu and directly uploading to colab session storage or by uploading to and mounting Google Drive

[5]:
```
from google.colab import files
files.upload()
```

```
<IPython.core.display.HTML object>
```

```
Saving alanine-dipeptide-0-250ns-nowater.xtc to alanine-dipeptide-0-250ns-
nowater.xtc
```

2.1 Install necessary packages (~10 mins)

[4]:
```
%pip install numpy scipy pandas scikit-learn jupyter ipywidgets==7.7.2␣
↪widgetsnbextension jupyter_contrib_nbextensions matplotlib MDTraj tqdm␣
↪pytest pyemma deeptime einops torch torchvision pytorch-lightning nglview
```

```
Requirement already satisfied: numpy in /usr/local/lib/python3.10/dist-packages
(1.25.2)
Requirement already satisfied: scipy in /usr/local/lib/python3.10/dist-packages
(1.11.4)
Requirement already satisfied: pandas in /usr/local/lib/python3.10/dist-packages
(2.0.3)
Requirement already satisfied: scikit-learn in /usr/local/lib/python3.10/dist-
packages (1.2.2)
Collecting jupyter
  Downloading jupyter-1.0.0-py2.py3-none-any.whl (2.7 kB)
Collecting ipywidgets==7.7.2
  Downloading ipywidgets-7.7.2-py2.py3-none-any.whl (123 kB)
                             123.4/123.4
kB 3.7 MB/s eta 0:00:00
Requirement already satisfied: widgetsnbextension in
/usr/local/lib/python3.10/dist-packages (3.6.6)
Collecting jupyter_contrib_nbextensions
  Downloading jupyter_contrib_nbextensions-0.7.0.tar.gz (23.5 MB)
                             23.5/23.5 MB
51.6 MB/s eta 0:00:00
  Preparing metadata (setup.py) … done
Requirement already satisfied: matplotlib in /usr/local/lib/python3.10/dist-
packages (3.7.1)
Collecting MDTraj
  Downloading mdtraj-1.9.9.tar.gz (2.2 MB)
                             2.2/2.2 MB
88.7 MB/s eta 0:00:00
  Installing build dependencies … done
  Getting requirements to build wheel … done
```

```
  Preparing metadata (pyproject.toml) … done
Requirement already satisfied: tqdm in /usr/local/lib/python3.10/dist-packages
(4.66.2)
Requirement already satisfied: pytest in /usr/local/lib/python3.10/dist-packages
(7.4.4)
Collecting pyemma
  Downloading pyEMMA-2.5.12.tar.gz (1.3 MB)
                             1.3/1.3 MB
84.4 MB/s eta 0:00:00
  Installing build dependencies … done
  Getting requirements to build wheel … done
  Preparing metadata (pyproject.toml) … done
Collecting deeptime
  Using cached
deeptime-0.4.4-cp310-cp310-manylinux_2_17_x86_64.manylinux2014_x86_64.whl (2.1
MB)
Collecting einops
  Downloading einops-0.8.0-py3-none-any.whl (43 kB)
                             43.2/43.2 kB
6.2 MB/s eta 0:00:00
Requirement already satisfied: torch in /usr/local/lib/python3.10/dist-
packages (2.2.1+cu121)
Requirement already satisfied: torchvision in /usr/local/lib/python3.10/dist-
packages (0.17.1+cu121)
Collecting pytorch-lightning
  Downloading pytorch_lightning-2.2.3-py3-none-any.whl (802 kB)
                             802.2/802.2
kB 70.4 MB/s eta 0:00:00
Collecting nglview
  Downloading nglview-3.1.2.tar.gz (5.5 MB)
                             5.5/5.5 MB
91.4 MB/s eta 0:00:00
  Installing build dependencies … done
  Getting requirements to build wheel … done
  Preparing metadata (pyproject.toml) … done
Requirement already satisfied: ipykernel>=4.5.1 in
/usr/local/lib/python3.10/dist-packages (from ipywidgets==7.7.2) (5.5.6)
Requirement already satisfied: ipython-genutils~=0.2.0 in
/usr/local/lib/python3.10/dist-packages (from ipywidgets==7.7.2) (0.2.0)
Requirement already satisfied: traitlets>=4.3.1 in
/usr/local/lib/python3.10/dist-packages (from ipywidgets==7.7.2) (5.7.1)
Requirement already satisfied: ipython>=4.0.0 in /usr/local/lib/python3.10/dist-
packages (from ipywidgets==7.7.2) (7.34.0)
Collecting jupyterlab-widgets<3,>=1.0.0 (from ipywidgets==7.7.2)
  Downloading jupyterlab_widgets-1.1.7-py3-none-any.whl (295 kB)
                             295.4/295.4
kB 25.0 MB/s eta 0:00:00
```

```
Requirement already satisfied: python-dateutil>=2.8.2 in
/usr/local/lib/python3.10/dist-packages (from pandas) (2.8.2)
Requirement already satisfied: pytz>=2020.1 in /usr/local/lib/python3.10/dist-
packages (from pandas) (2023.4)
Requirement already satisfied: tzdata>=2022.1 in /usr/local/lib/python3.10/dist-
packages (from pandas) (2024.1)
Requirement already satisfied: joblib>=1.1.1 in /usr/local/lib/python3.10/dist-
packages (from scikit-learn) (1.4.0)
Requirement already satisfied: threadpoolctl>=2.0.0 in
/usr/local/lib/python3.10/dist-packages (from scikit-learn) (3.4.0)
Requirement already satisfied: notebook in /usr/local/lib/python3.10/dist-
packages (from jupyter) (6.5.5)
Collecting qtconsole (from jupyter)
  Downloading qtconsole-5.5.1-py3-none-any.whl (123 kB)
                            123.4/123.4
kB 18.8 MB/s eta 0:00:00
Requirement already satisfied: jupyter-console in
/usr/local/lib/python3.10/dist-packages (from jupyter) (6.1.0)
Requirement already satisfied: nbconvert in /usr/local/lib/python3.10/dist-
packages (from jupyter) (6.5.4)
Collecting jupyter_contrib_core>=0.3.3 (from jupyter_contrib_nbextensions)
  Downloading jupyter_contrib_core-0.4.2.tar.gz (17 kB)
  Preparing metadata (setup.py) … done
Requirement already satisfied: jupyter_core in /usr/local/lib/python3.10/dist-
packages (from jupyter_contrib_nbextensions) (5.7.2)
Collecting jupyter_highlight_selected_word>=0.1.1 (from
jupyter_contrib_nbextensions)
  Downloading jupyter_highlight_selected_word-0.2.0-py2.py3-none-any.whl (11 kB)
Collecting jupyter_nbextensions_configurator>=0.4.0 (from
jupyter_contrib_nbextensions)
  Downloading jupyter_nbextensions_configurator-0.6.3-py2.py3-none-any.whl (466
kB)
                            466.9/466.9
kB 47.9 MB/s eta 0:00:00
Requirement already satisfied: tornado in /usr/local/lib/python3.10/dist-
packages (from jupyter_contrib_nbextensions) (6.3.3)
Requirement already satisfied: lxml in /usr/local/lib/python3.10/dist-packages
(from jupyter_contrib_nbextensions) (4.9.4)
Requirement already satisfied: contourpy>=1.0.1 in
/usr/local/lib/python3.10/dist-packages (from matplotlib) (1.2.1)
Requirement already satisfied: cycler>=0.10 in /usr/local/lib/python3.10/dist-
packages (from matplotlib) (0.12.1)
Requirement already satisfied: fonttools>=4.22.0 in
/usr/local/lib/python3.10/dist-packages (from matplotlib) (4.51.0)
Requirement already satisfied: kiwisolver>=1.0.1 in
/usr/local/lib/python3.10/dist-packages (from matplotlib) (1.4.5)
```

```
Requirement already satisfied: packaging>=20.0 in
/usr/local/lib/python3.10/dist-packages (from matplotlib) (24.0)
Requirement already satisfied: pillow>=6.2.0 in /usr/local/lib/python3.10/dist-
packages (from matplotlib) (9.4.0)
Requirement already satisfied: pyparsing>=2.3.1 in
/usr/local/lib/python3.10/dist-packages (from matplotlib) (3.1.2)
Requirement already satisfied: astunparse in /usr/local/lib/python3.10/dist-
packages (from MDTraj) (1.6.3)
Requirement already satisfied: iniconfig in /usr/local/lib/python3.10/dist-
packages (from pytest) (2.0.0)
Requirement already satisfied: pluggy<2.0,>=0.12 in
/usr/local/lib/python3.10/dist-packages (from pytest) (1.5.0)
Requirement already satisfied: exceptiongroup>=1.0.0rc8 in
/usr/local/lib/python3.10/dist-packages (from pytest) (1.2.1)
Requirement already satisfied: tomli>=1.0.0 in /usr/local/lib/python3.10/dist-
packages (from pytest) (2.0.1)
Requirement already satisfied: decorator>=4.0.0 in
/usr/local/lib/python3.10/dist-packages (from pyemma) (4.4.2)
Requirement already satisfied: h5py>=2.7.1 in /usr/local/lib/python3.10/dist-
packages (from pyemma) (3.9.0)
Collecting pathos (from pyemma)
  Downloading pathos-0.3.2-py3-none-any.whl (82 kB)
                           82.1/82.1 kB
12.5 MB/s eta 0:00:00
Requirement already satisfied: psutil>=3.1.1 in
/usr/local/lib/python3.10/dist-packages (from pyemma) (5.9.5)
Requirement already satisfied: pyyaml in /usr/local/lib/python3.10/dist-packages
(from pyemma) (6.0.1)
Requirement already satisfied: filelock in /usr/local/lib/python3.10/dist-
packages (from torch) (3.13.4)
Requirement already satisfied: typing-extensions>=4.8.0 in
/usr/local/lib/python3.10/dist-packages (from torch) (4.11.0)
Requirement already satisfied: sympy in /usr/local/lib/python3.10/dist-packages
(from torch) (1.12)
Requirement already satisfied: networkx in /usr/local/lib/python3.10/dist-
packages (from torch) (3.3)
Requirement already satisfied: jinja2 in /usr/local/lib/python3.10/dist-packages
(from torch) (3.1.3)
Requirement already satisfied: fsspec in /usr/local/lib/python3.10/dist-packages
(from torch) (2023.6.0)
Collecting nvidia-cuda-nvrtc-cu12==12.1.105 (from torch)
  Using cached nvidia_cuda_nvrtc_cu12-12.1.105-py3-none-manylinux1_x86_64.whl
(23.7 MB)
Collecting nvidia-cuda-runtime-cu12==12.1.105 (from torch)
  Using cached nvidia_cuda_runtime_cu12-12.1.105-py3-none-manylinux1_x86_64.whl
(823 kB)
Collecting nvidia-cuda-cupti-cu12==12.1.105 (from torch)
  Using cached nvidia_cuda_cupti_cu12-12.1.105-py3-none-manylinux1_x86_64.whl
```

```
(14.1 MB)
Collecting nvidia-cudnn-cu12==8.9.2.26 (from torch)
  Using cached nvidia_cudnn_cu12-8.9.2.26-py3-none-manylinux1_x86_64.whl (731.7
MB)
Collecting nvidia-cublas-cu12==12.1.3.1 (from torch)
  Using cached nvidia_cublas_cu12-12.1.3.1-py3-none-manylinux1_x86_64.whl (410.6
MB)
Collecting nvidia-cufft-cu12==11.0.2.54 (from torch)
  Using cached nvidia_cufft_cu12-11.0.2.54-py3-none-manylinux1_x86_64.whl (121.6
MB)
Collecting nvidia-curand-cu12==10.3.2.106 (from torch)
  Using cached nvidia_curand_cu12-10.3.2.106-py3-none-manylinux1_x86_64.whl
(56.5 MB)
Collecting nvidia-cusolver-cu12==11.4.5.107 (from torch)
  Using cached nvidia_cusolver_cu12-11.4.5.107-py3-none-manylinux1_x86_64.whl
(124.2 MB)
Collecting nvidia-cusparse-cu12==12.1.0.106 (from torch)
  Using cached nvidia_cusparse_cu12-12.1.0.106-py3-none-manylinux1_x86_64.whl
(196.0 MB)
Collecting nvidia-nccl-cu12==2.19.3 (from torch)
  Using cached nvidia_nccl_cu12-2.19.3-py3-none-manylinux1_x86_64.whl (166.0 MB)
Collecting nvidia-nvtx-cu12==12.1.105 (from torch)
  Using cached nvidia_nvtx_cu12-12.1.105-py3-none-manylinux1_x86_64.whl (99 kB)
Requirement already satisfied: triton==2.2.0 in /usr/local/lib/python3.10/dist-
packages (from torch) (2.2.0)
Collecting nvidia-nvjitlink-cu12 (from nvidia-cusolver-cu12==11.4.5.107->torch)
  Using cached nvidia_nvjitlink_cu12-12.4.127-py3-none-manylinux2014_x86_64.whl
(21.1 MB)
Collecting torchmetrics>=0.7.0 (from pytorch-lightning)
  Downloading torchmetrics-1.3.2-py3-none-any.whl (841 kB)
                             841.5/841.5
kB 62.1 MB/s eta 0:00:00
Collecting lightning-utilities>=0.8.0 (from pytorch-lightning)
  Downloading lightning_utilities-0.11.2-py3-none-any.whl (26 kB)
INFO: pip is looking at multiple versions of nglview to determine which version
is compatible with other requirements. This could take a while.
Collecting nglview
  Downloading nglview-3.1.1.tar.gz (5.5 MB)
                             5.5/5.5 MB
105.0 MB/s eta 0:00:00
  Installing build dependencies … done
  Getting requirements to build wheel … done
  Preparing metadata (pyproject.toml) … done
  Downloading nglview-3.1.0.tar.gz (5.5 MB)
                             5.5/5.5 MB
106.2 MB/s eta 0:00:00
  Installing build dependencies … done
```

```
  Getting requirements to build wheel … done
  Preparing metadata (pyproject.toml) … done
  Downloading nglview-3.0.8.tar.gz (6.8 MB)
                             6.8/6.8 MB
110.7 MB/s eta 0:00:00
  Installing build dependencies … done
  Getting requirements to build wheel … done
  Preparing metadata (pyproject.toml) … done
Requirement already satisfied: requests in /usr/local/lib/python3.10/dist-
packages (from fsspec->torch) (2.31.0)
Requirement already satisfied: aiohttp!=4.0.0a0,!=4.0.0a1 in
/usr/local/lib/python3.10/dist-packages (from fsspec->torch) (3.9.5)
Requirement already satisfied: jupyter-client in /usr/local/lib/python3.10/dist-
packages (from ipykernel>=4.5.1->ipywidgets==7.7.2) (6.1.12)
Requirement already satisfied: setuptools>=18.5 in
/usr/local/lib/python3.10/dist-packages (from ipython>=4.0.0->ipywidgets==7.7.2)
(67.7.2)
Collecting jedi>=0.16 (from ipython>=4.0.0->ipywidgets==7.7.2)
  Downloading jedi-0.19.1-py2.py3-none-any.whl (1.6 MB)
                             1.6/1.6 MB
71.0 MB/s eta 0:00:00
Requirement already satisfied: pickleshare in
/usr/local/lib/python3.10/dist-packages (from ipython>=4.0.0->ipywidgets==7.7.2)
(0.7.5)
Requirement already satisfied: prompt-toolkit!=3.0.0,!=3.0.1,<3.1.0,>=2.0.0 in
/usr/local/lib/python3.10/dist-packages (from ipython>=4.0.0->ipywidgets==7.7.2)
(3.0.43)
Requirement already satisfied: pygments in /usr/local/lib/python3.10/dist-
packages (from ipython>=4.0.0->ipywidgets==7.7.2) (2.16.1)
Requirement already satisfied: backcall in /usr/local/lib/python3.10/dist-
packages (from ipython>=4.0.0->ipywidgets==7.7.2) (0.2.0)
Requirement already satisfied: matplotlib-inline in
/usr/local/lib/python3.10/dist-packages (from ipython>=4.0.0->ipywidgets==7.7.2)
(0.1.7)
Requirement already satisfied: pexpect>4.3 in /usr/local/lib/python3.10/dist-
packages (from ipython>=4.0.0->ipywidgets==7.7.2) (4.9.0)
Requirement already satisfied: beautifulsoup4 in /usr/local/lib/python3.10/dist-
packages (from nbconvert->jupyter) (4.12.3)
Requirement already satisfied: bleach in /usr/local/lib/python3.10/dist-packages
(from nbconvert->jupyter) (6.1.0)
Requirement already satisfied: defusedxml in /usr/local/lib/python3.10/dist-
packages (from nbconvert->jupyter) (0.7.1)
Requirement already satisfied: entrypoints>=0.2.2 in
/usr/local/lib/python3.10/dist-packages (from nbconvert->jupyter) (0.4)
Requirement already satisfied: jupyterlab-pygments in
/usr/local/lib/python3.10/dist-packages (from nbconvert->jupyter) (0.3.0)
Requirement already satisfied: MarkupSafe>=2.0 in
/usr/local/lib/python3.10/dist-packages (from nbconvert->jupyter) (2.1.5)
```

```
Requirement already satisfied: mistune<2,>=0.8.1 in
/usr/local/lib/python3.10/dist-packages (from nbconvert->jupyter) (0.8.4)
Requirement already satisfied: nbclient>=0.5.0 in
/usr/local/lib/python3.10/dist-packages (from nbconvert->jupyter) (0.10.0)
Requirement already satisfied: nbformat>=5.1 in /usr/local/lib/python3.10/dist-
packages (from nbconvert->jupyter) (5.10.4)
Requirement already satisfied: pandocfilters>=1.4.1 in
/usr/local/lib/python3.10/dist-packages (from nbconvert->jupyter) (1.5.1)
Requirement already satisfied: tinycss2 in /usr/local/lib/python3.10/dist-
packages (from nbconvert->jupyter) (1.2.1)
Requirement already satisfied: platformdirs>=2.5 in
/usr/local/lib/python3.10/dist-packages (from
jupyter_core->jupyter_contrib_nbextensions) (4.2.0)
Requirement already satisfied: pyzmq<25,>=17 in /usr/local/lib/python3.10/dist-
packages (from notebook->jupyter) (23.2.1)
Requirement already satisfied: argon2-cffi in /usr/local/lib/python3.10/dist-
packages (from notebook->jupyter) (23.1.0)
Requirement already satisfied: nest-asyncio>=1.5 in
/usr/local/lib/python3.10/dist-packages (from notebook->jupyter) (1.6.0)
Requirement already satisfied: Send2Trash>=1.8.0 in
/usr/local/lib/python3.10/dist-packages (from notebook->jupyter) (1.8.3)
Requirement already satisfied: terminado>=0.8.3 in
/usr/local/lib/python3.10/dist-packages (from notebook->jupyter) (0.18.1)
Requirement already satisfied: prometheus-client in
/usr/local/lib/python3.10/dist-packages (from notebook->jupyter) (0.20.0)
Requirement already satisfied: nbclassic>=0.4.7 in
/usr/local/lib/python3.10/dist-packages (from notebook->jupyter) (1.0.0)
Requirement already satisfied: six>=1.5 in /usr/local/lib/python3.10/dist-
packages (from python-dateutil>=2.8.2->pandas) (1.16.0)
Requirement already satisfied: wheel<1.0,>=0.23.0 in
/usr/local/lib/python3.10/dist-packages (from astunparse->MDTraj) (0.43.0)
Collecting ppft>=1.7.6.8 (from pathos->pyemma)
  Downloading ppft-1.7.6.8-py3-none-any.whl (56 kB)
                           56.8/56.8 kB
8.8 MB/s eta 0:00:00
Collecting dill>=0.3.8 (from pathos->pyemma)
  Downloading dill-0.3.8-py3-none-any.whl (116 kB)
                           116.3/116.3

kB 19.3 MB/s eta 0:00:00
Collecting pox>=0.3.4 (from pathos->pyemma)
  Downloading pox-0.3.4-py3-none-any.whl (29 kB)
Collecting multiprocess>=0.70.16 (from pathos->pyemma)
  Downloading multiprocess-0.70.16-py310-none-any.whl (134 kB)
                           134.8/134.8

kB 20.1 MB/s eta 0:00:00
Collecting qtpy>=2.4.0 (from qtconsole->jupyter)
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  Downloading QtPy-2.4.1-py3-none-any.whl (93 kB)
                             93.5/93.5 kB
13.9 MB/s eta 0:00:00
Requirement already satisfied: mpmath>=0.19 in
/usr/local/lib/python3.10/dist-packages (from sympy->torch) (1.3.0)
Requirement already satisfied: aiosignal>=1.1.2 in
/usr/local/lib/python3.10/dist-packages (from
aiohttp!=4.0.0a0,!=4.0.0a1->fsspec->torch) (1.3.1)
Requirement already satisfied: attrs>=17.3.0 in /usr/local/lib/python3.10/dist-
packages (from aiohttp!=4.0.0a0,!=4.0.0a1->fsspec->torch) (23.2.0)
Requirement already satisfied: frozenlist>=1.1.1 in
/usr/local/lib/python3.10/dist-packages (from
aiohttp!=4.0.0a0,!=4.0.0a1->fsspec->torch) (1.4.1)
Requirement already satisfied: multidict<7.0,>=4.5 in
/usr/local/lib/python3.10/dist-packages (from
aiohttp!=4.0.0a0,!=4.0.0a1->fsspec->torch) (6.0.5)
Requirement already satisfied: yarl<2.0,>=1.0 in /usr/local/lib/python3.10/dist-
packages (from aiohttp!=4.0.0a0,!=4.0.0a1->fsspec->torch) (1.9.4)
Requirement already satisfied: async-timeout<5.0,>=4.0 in
/usr/local/lib/python3.10/dist-packages (from
aiohttp!=4.0.0a0,!=4.0.0a1->fsspec->torch) (4.0.3)
Requirement already satisfied: parso<0.9.0,>=0.8.3 in
/usr/local/lib/python3.10/dist-packages (from
jedi>=0.16->ipython>=4.0.0->ipywidgets==7.7.2) (0.8.4)
Requirement already satisfied: jupyter-server>=1.8 in
/usr/local/lib/python3.10/dist-packages (from
nbclassic>=0.4.7->notebook->jupyter) (1.24.0)
Requirement already satisfied: notebook-shim>=0.2.3 in
/usr/local/lib/python3.10/dist-packages (from
nbclassic>=0.4.7->notebook->jupyter) (0.2.4)
Requirement already satisfied: fastjsonschema>=2.15 in
/usr/local/lib/python3.10/dist-packages (from nbformat>=5.1->nbconvert->jupyter)
(2.19.1)
Requirement already satisfied: jsonschema>=2.6 in
/usr/local/lib/python3.10/dist-packages (from nbformat>=5.1->nbconvert->jupyter)
(4.19.2)
Requirement already satisfied: ptyprocess>=0.5 in
/usr/local/lib/python3.10/dist-packages (from
pexpect>4.3->ipython>=4.0.0->ipywidgets==7.7.2) (0.7.0)
Requirement already satisfied: wcwidth in /usr/local/lib/python3.10/dist-
packages (from prompt-
toolkit!=3.0.0,!=3.0.1,<3.1.0,>=2.0.0->ipython>=4.0.0->ipywidgets==7.7.2)
(0.2.13)
Requirement already satisfied: argon2-cffi-bindings in
/usr/local/lib/python3.10/dist-packages (from argon2-cffi->notebook->jupyter)
(21.2.0)
Requirement already satisfied: soupsieve>1.2 in /usr/local/lib/python3.10/dist-
packages (from beautifulsoup4->nbconvert->jupyter) (2.5)
```

```
Requirement already satisfied: webencodings in /usr/local/lib/python3.10/dist-
packages (from bleach->nbconvert->jupyter) (0.5.1)
Requirement already satisfied: charset-normalizer<4,>=2 in
/usr/local/lib/python3.10/dist-packages (from requests->fsspec->torch) (3.3.2)
Requirement already satisfied: idna<4,>=2.5 in /usr/local/lib/python3.10/dist-
packages (from requests->fsspec->torch) (3.7)
Requirement already satisfied: urllib3<3,>=1.21.1 in
/usr/local/lib/python3.10/dist-packages (from requests->fsspec->torch) (2.0.7)
Requirement already satisfied: certifi>=2017.4.17 in
/usr/local/lib/python3.10/dist-packages (from requests->fsspec->torch)
(2024.2.2)
Requirement already satisfied: jsonschema-specifications>=2023.03.6 in
/usr/local/lib/python3.10/dist-packages (from
jsonschema>=2.6->nbformat>=5.1->nbconvert->jupyter) (2023.12.1)
Requirement already satisfied: referencing>=0.28.4 in
/usr/local/lib/python3.10/dist-packages (from
jsonschema>=2.6->nbformat>=5.1->nbconvert->jupyter) (0.34.0)
Requirement already satisfied: rpds-py>=0.7.1 in /usr/local/lib/python3.10/dist-
packages (from jsonschema>=2.6->nbformat>=5.1->nbconvert->jupyter) (0.18.0)
Requirement already satisfied: anyio<4,>=3.1.0 in
/usr/local/lib/python3.10/dist-packages (from jupyter-
server>=1.8->nbclassic>=0.4.7->notebook->jupyter) (3.7.1)
Requirement already satisfied: websocket-client in
/usr/local/lib/python3.10/dist-packages (from jupyter-
server>=1.8->nbclassic>=0.4.7->notebook->jupyter) (1.7.0)
Requirement already satisfied: cffi>=1.0.1 in /usr/local/lib/python3.10/dist-
packages (from argon2-cffi-bindings->argon2-cffi->notebook->jupyter) (1.16.0)
Requirement already satisfied: sniffio>=1.1 in /usr/local/lib/python3.10/dist-
packages (from anyio<4,>=3.1.0->jupyter-
server>=1.8->nbclassic>=0.4.7->notebook->jupyter) (1.3.1)
Requirement already satisfied: pycparser in /usr/local/lib/python3.10/dist-
packages (from cffi>=1.0.1->argon2-cffi-
bindings->argon2-cffi->notebook->jupyter) (2.22)
Building wheels for collected packages: jupyter_contrib_nbextensions, MDTraj,
pyemma, nglview, jupyter_contrib_core
  Building wheel for jupyter_contrib_nbextensions (setup.py) …
done
  Created wheel for jupyter_contrib_nbextensions:
filename=jupyter_contrib_nbextensions-0.7.0-py2.py3-none-any.whl size=23428780
sha256=54c5bd7f3580944a65ca0e10aaa94eb282d00aa1b742f1e7d11cf44cf7ee970e
  Stored in directory: /root/.cache/pip/wheels/ea/cc/7d/99ef154f984726b1201c0f72
cfe9c9d7c5132c1a2ae4d8677f
  Building wheel for MDTraj (pyproject.toml) … done
  Created wheel for MDTraj: filename=mdtraj-1.9.9-cp310-cp310-linux_x86_64.whl
size=7547268
sha256=32e1bb5de92bfa09a7e15562b9bdc207c5e9806ed44e24b16c443424f6a12535
  Stored in directory: /root/.cache/pip/wheels/4b/4e/d5/22b44e04aca0780281ffb437
17ebb3404bc1a77cf8f345fa73
```

```
  Building wheel for pyemma (pyproject.toml) … done
  Created wheel for pyemma: filename=pyEMMA-2.5.12-cp310-cp310-linux_x86_64.whl
size=2712144
sha256=77d1627e2b6239996c731a801f7e0115fec28a95d27f50ca5677443a47be668c
  Stored in directory: /root/.cache/pip/wheels/26/e7/52/8fcd9a27e834967fc71dedff
33de9038999783184ec26af7a6
  Building wheel for nglview (pyproject.toml) … done
  Created wheel for nglview: filename=nglview-3.0.8-py3-none-any.whl
size=10216160
sha256=4961aae9cdfc33205c4ada655e58fdcb02fece4057ca67febf30b5cf7e8b4975
  Stored in directory: /root/.cache/pip/wheels/2e/6c/59/32bf4aa0134f9c4cdca054f5
192839fb4285241e2f17f7d358
  Building wheel for jupyter_contrib_core (setup.py) … done
  Created wheel for jupyter_contrib_core:
filename=jupyter_contrib_core-0.4.2-py2.py3-none-any.whl size=17482
sha256=957d5f23214f03657886c7320d61c13149dadbe9420b613d36cc71066e37d46b
  Stored in directory: /root/.cache/pip/wheels/a9/52/88/e0643cdfd68f0562087918c3
7dd583378648dbc3df68b907f7
Successfully built jupyter_contrib_nbextensions MDTraj pyemma nglview
jupyter_contrib_core
Installing collected packages: jupyter_highlight_selected_word, qtpy, ppft, pox,
nvidia-nvtx-cu12, nvidia-nvjitlink-cu12, nvidia-nccl-cu12, nvidia-curand-cu12,
nvidia-cufft-cu12, nvidia-cuda-runtime-cu12, nvidia-cuda-nvrtc-cu12, nvidia-
cuda-cupti-cu12, nvidia-cublas-cu12, lightning-utilities, jupyterlab-widgets,
jedi, einops, dill, nvidia-cusparse-cu12, nvidia-cudnn-cu12, multiprocess,
MDTraj, pathos, nvidia-cusolver-cu12, deeptime, qtconsole, pyemma, torchmetrics,
pytorch-lightning, jupyter_contrib_core, jupyter_nbextensions_configurator,
ipywidgets, nglview, jupyter_contrib_nbextensions, jupyter
  Attempting uninstall: jupyterlab-widgets
    Found existing installation: jupyterlab_widgets 3.0.10
    Uninstalling jupyterlab_widgets-3.0.10:
      Successfully uninstalled jupyterlab_widgets-3.0.10
  Attempting uninstall: ipywidgets
    Found existing installation: ipywidgets 7.7.1
    Uninstalling ipywidgets-7.7.1:
      Successfully uninstalled ipywidgets-7.7.1
Successfully installed MDTraj-1.9.9 deeptime-0.4.4 dill-0.3.8 einops-0.8.0
ipywidgets-7.7.2 jedi-0.19.1 jupyter-1.0.0 jupyter_contrib_core-0.4.2
jupyter_contrib_nbextensions-0.7.0 jupyter_highlight_selected_word-0.2.0
jupyter_nbextensions_configurator-0.6.3 jupyterlab-widgets-1.1.7 lightning-
utilities-0.11.2 multiprocess-0.70.16 nglview-3.0.8 nvidia-cublas-cu12-12.1.3.1
nvidia-cuda-cupti-cu12-12.1.105 nvidia-cuda-nvrtc-cu12-12.1.105 nvidia-cuda-
runtime-cu12-12.1.105 nvidia-cudnn-cu12-8.9.2.26 nvidia-cufft-cu12-11.0.2.54
nvidia-curand-cu12-10.3.2.106 nvidia-cusolver-cu12-11.4.5.107 nvidia-cusparse-
cu12-12.1.0.106 nvidia-nccl-cu12-2.19.3 nvidia-nvjitlink-cu12-12.4.127 nvidia-
nvtx-cu12-12.1.105 pathos-0.3.2 pox-0.3.4 ppft-1.7.6.8 pyemma-2.5.12 pytorch-
lightning-2.2.3 qtconsole-5.5.1 qtpy-2.4.1 torchmetrics-1.3.2
```

[6]:
```
!jupyter nbextension enable --py --sys-prefix widgetsnbextension
```

```
Enabling notebook extension jupyter-js-widgets/extension…
Paths used for configuration of notebook:
        /usr/etc/jupyter/nbconfig/notebook.json
Paths used for configuration of notebook:

      - Validating: OK
Paths used for configuration of notebook:
        /usr/etc/jupyter/nbconfig/notebook.json
```

[7]:
```
!jupyter nbextension enable nglview --py --sys-prefix
```

```
Enabling notebook extension nglview-js-widgets/extension…
Paths used for configuration of notebook:
        /usr/etc/jupyter/nbconfig/notebook.json
Paths used for configuration of notebook:

      - Validating: OK
Paths used for configuration of notebook:
        /usr/etc/jupyter/nbconfig/notebook.json
```

[8]:
```
!nglview enable
```

```
Enabling notebook extension nglview-js-widgets/extension…
Paths used for configuration of notebook:
        /usr/etc/jupyter/nbconfig/notebook.json
Paths used for configuration of notebook:

      - Validating: OK
Paths used for configuration of notebook:
        /usr/etc/jupyter/nbconfig/notebook.json
```

[9]:
```
%pip install git+https://github.com/andrewlferguson/snrv.git
```

```
Collecting git+https://github.com/andrewlferguson/snrv.git
  Cloning https://github.com/andrewlferguson/snrv.git to /tmp/pip-req-
build-5kuoreb9
  Running command git clone --filter=blob:none --quiet
https://github.com/andrewlferguson/snrv.git /tmp/pip-req-build-5kuoreb9
  Resolved https://github.com/andrewlferguson/snrv.git to commit
63aeebc2f0253bec9f5e0ab03615c107256bf34f
  Preparing metadata (setup.py) … done
Building wheels for collected packages: snrv
  Building wheel for snrv (setup.py) … done
  Created wheel for snrv: filename=snrv-0.1.0+52.g63aeebc-py3-none-any.whl
size=30278
sha256=783c495dc695ac66886bbfe71cd357738c2b9b44080945d7ffb50511f03da77f
```

```
  Stored in directory: /tmp/pip-ephem-wheel-cache-
bvft170g/wheels/d8/83/c6/26e7926d23676778257c4238a0e7ca498b668f07b425672242
Successfully built snrv
Installing collected packages: snrv
Successfully installed snrv-0.1.0+52.g63aeebc
```

[10]:
```
%pip install git+https://github.com/Ferg-Lab/mdn_propagator.git
```

```
Collecting git+https://github.com/Ferg-Lab/mdn_propagator.git
  Cloning https://github.com/Ferg-Lab/mdn_propagator.git to /tmp/pip-req-build-
jm9h7_u2
  Running command git clone --filter=blob:none --quiet https://github.com/Ferg-
Lab/mdn_propagator.git /tmp/pip-req-build-jm9h7_u2
  Resolved https://github.com/Ferg-Lab/mdn_propagator.git to commit
ad8fd32faf84908b2c4f58bf7e16195a7c4f29e8
  Installing build dependencies … done
  Getting requirements to build wheel … done
  Installing backend dependencies … done
  Preparing metadata (pyproject.toml) … done
Building wheels for collected packages: mdn_propagator
  Building wheel for mdn_propagator (pyproject.toml) … done
  Created wheel for mdn_propagator:
filename=mdn_propagator-1.0.0+32.gad8fd32-py3-none-any.whl size=15911
sha256=1a9f05c32d3243520a6373a2fd5d9b077eceda6e26e99925c21c1e640a1e7262
  Stored in directory: /tmp/pip-ephem-wheel-cache-n7vhvnqz/wheels/bc/a7/ff/4f2aa
2dbe5dc942686e82380dbec7ba232e35df5f5213de831
Successfully built mdn_propagator
Installing collected packages: mdn_propagator
Successfully installed mdn_propagator-1.0.0+32.gad8fd32
```

[11]:
```
%pip install git+https://github.com/Ferg-Lab/molgen.git
```

```
Collecting git+https://github.com/Ferg-Lab/molgen.git
  Cloning https://github.com/Ferg-Lab/molgen.git to /tmp/pip-req-build-ia6k6i_r
  Running command git clone --filter=blob:none --quiet https://github.com/Ferg-
Lab/molgen.git /tmp/pip-req-build-ia6k6i_r
  Resolved https://github.com/Ferg-Lab/molgen.git to commit
533a1ccbcd5d59d5beea36d26a68ff4e6c28816c
  Installing build dependencies … done
  Getting requirements to build wheel … done
  Installing backend dependencies … done
  Preparing metadata (pyproject.toml) … done
Building wheels for collected packages: molgen
  Building wheel for molgen (pyproject.toml) … done
  Created wheel for molgen: filename=molgen-1.0.0+15.g533a1cc-py3-none-any.whl
size=20455
sha256=f387b319ded3f25fcc7bb718006ad88280b2d3ddd567f203d9c7a79c42ababbd
  Stored in directory: /tmp/pip-ephem-wheel-cache-
```

```
ty1nv6df/wheels/1e/82/fb/a86e30e540a9156a4dfcf1eb19c92a23f5b728019e949672b1
Successfully built molgen
Installing collected packages: molgen
Successfully installed molgen-1.0.0+15.g533a1cc
```

2.2 Load the different components from their respective repos (~1 min)

[12]:
```
from mdn_propagator.propagator import Propagator
from molgen.models import DDPM
from snrv import Snrv
from snrv.utils import set_random_seed
```

2.2.1 Other dependencies

[13]:
```
import mdtraj as md
from pathlib import Path
import torch
import matplotlib.pyplot as plt
import numpy as np
import nglview as nv
```

[14]:
```
from google.colab import output
output.enable_custom_widget_manager()
```

3 Load and prep data (~1 min)

[15]:
```
trj_fnames = sorted([str(i) for i in Path('./').
  ↪glob('alanine-dipeptide-*-250ns-nowater.xtc')])
top_fname = 'alanine-dipeptide-nowater.pdb'
```

[16]:
```
trjs = [md.load(t, top=top_fname).center_coordinates() for t in trj_fnames]
trjs
```

[16]:
```
[<mdtraj.Trajectory with 250000 frames, 22 atoms, 3 residues, and unitcells at
0x7b329c7677c0>]
```

[17]:
```
v = nv.show_mdtraj(trjs[0])
v
```

```
NGLWidget(max_frame=249999)
```

[18]:
```
coords_torch = list()
for trj in trjs:
    #t_backbone = trj.atom_slice(trj.top.select('backbone')).
 ↪center_coordinates()
    #pdists = [torch.pdist(p)[None] for p in torch.tensor(t_backbone.xyz)]
    pdists = [torch.pdist(p)[None] for p in torch.tensor(trj.xyz)]
    coords_torch.append(torch.cat(pdists))
len(coords_torch), coords_torch[0].shape
```

[18]:
```
(1, torch.Size([250000, 231]))
```

4 SRV fitting (~5 mins)

[19]:
```
set_random_seed(42)
```

```
Setting random seed to 42
```

[20]:
```
input_size = coords_torch[0].size()[1]
output_size = 3
hidden_depth = 2
hidden_size = 100
batch_norm = True
dropout_rate = 0.0
lr = 1E-2
weight_decay = 0.0
val_frac = 0.05
n_epochs = 30
batch_size = 25000
VAMPdegree = 2
is_reversible = True
num_workers = 0

model_snrv = Snrv(input_size, output_size, hidden_depth=hidden_depth,␣
 ↪hidden_size=hidden_size,
            batch_norm=batch_norm, dropout_rate=dropout_rate, lr=lr,␣
 ↪weight_decay=weight_decay,
            val_frac=val_frac, n_epochs=n_epochs, batch_size=batch_size,
            VAMPdegree=VAMPdegree,is_reversible=is_reversible,␣
 ↪num_workers=num_workers,
            activation=torch.nn.GELU(), device=device)
model_snrv = model_snrv.to(device)
```

[21]:
```
lag_n = 10
```

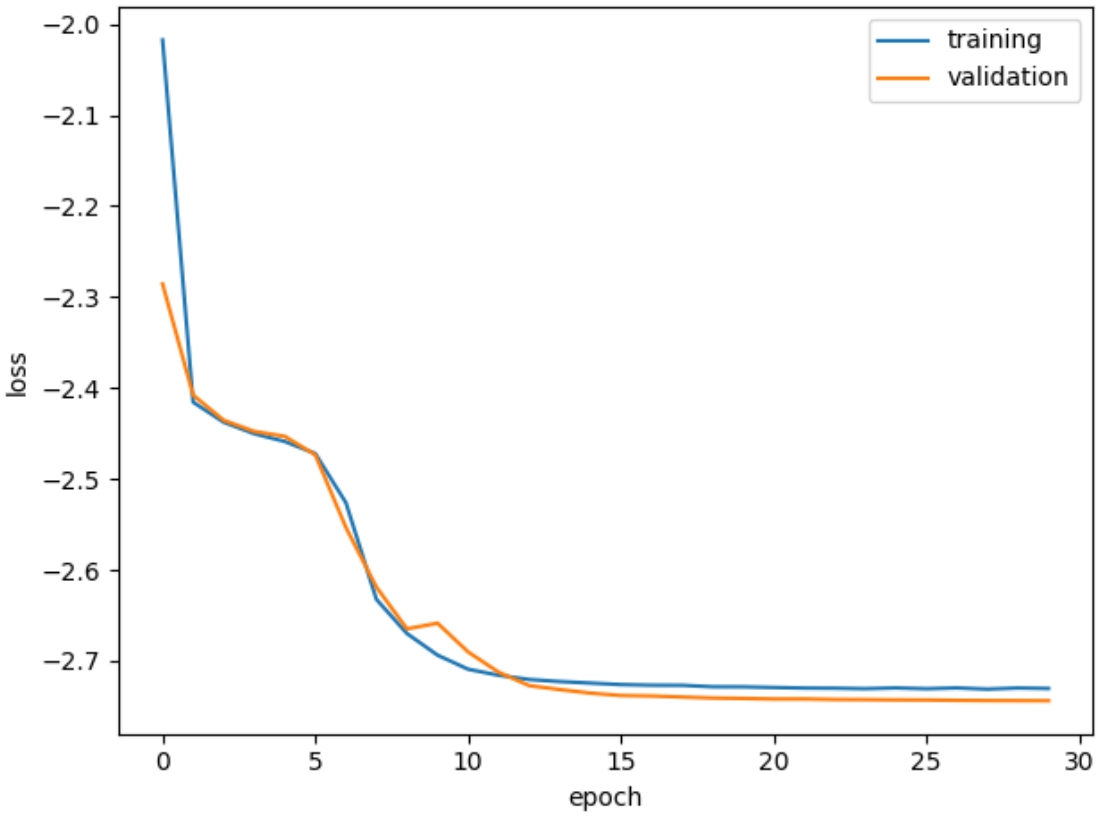
[22]:
```
model_snrv.fit(coords_torch, lag=lag_n, scheduler=0.9)
```

```
Epoch 0: 100%|     | 10/10 [00:05<00:00,  1.98batch/s]
[Epoch 0]        training loss = -2.017  validation loss = -2.286
Epoch 1: 100%|     | 10/10 [00:04<00:00,  2.50batch/s]
[Epoch 1]        training loss = -2.415  validation loss = -2.408
Epoch 2: 100%|     | 10/10 [00:04<00:00,  2.49batch/s]
[Epoch 2]        training loss = -2.438  validation loss = -2.435
Epoch 3: 100%|     | 10/10 [00:03<00:00,  2.52batch/s]
[Epoch 3]        training loss = -2.450  validation loss = -2.448
Epoch 4: 100%|     | 10/10 [00:03<00:00,  2.52batch/s]
[Epoch 4]        training loss = -2.459  validation loss = -2.453
Epoch 5: 100%|     | 10/10 [00:03<00:00,  2.52batch/s]
[Epoch 5]        training loss = -2.472  validation loss = -2.473
Epoch 6: 100%|     | 10/10 [00:03<00:00,  2.52batch/s]
[Epoch 6]        training loss = -2.526  validation loss = -2.553
Epoch 7: 100%|     | 10/10 [00:04<00:00,  2.49batch/s]
[Epoch 7]        training loss = -2.632  validation loss = -2.619
Epoch 8: 100%|     | 10/10 [00:03<00:00,  2.51batch/s]
[Epoch 8]        training loss = -2.670  validation loss = -2.665
Epoch 9: 100%|     | 10/10 [00:03<00:00,  2.50batch/s]
[Epoch 9]        training loss = -2.694  validation loss = -2.658
Epoch 10: 100%|     | 10/10 [00:04<00:00,  2.49batch/s]
[Epoch 10]       training loss = -2.709  validation loss = -2.690
Epoch 11: 100%|     | 10/10 [00:04<00:00,  2.49batch/s]
[Epoch 11]       training loss = -2.716  validation loss = -2.712
Epoch 12: 100%|     | 10/10 [00:04<00:00,  2.49batch/s]
[Epoch 12]       training loss = -2.720  validation loss = -2.727
Epoch 13: 100%|     | 10/10 [00:04<00:00,  2.47batch/s]
[Epoch 13]       training loss = -2.723  validation loss = -2.731
Epoch 14: 100%|     | 10/10 [00:04<00:00,  2.48batch/s]
[Epoch 14]       training loss = -2.724  validation loss = -2.735
Epoch 15: 100%|     | 10/10 [00:04<00:00,  2.48batch/s]
[Epoch 15]       training loss = -2.726  validation loss = -2.738
```

```
Epoch 16: 100%|     | 10/10 [00:04<00:00,  2.49batch/s]
[Epoch 16]       training loss = -2.727  validation loss = -2.738
Epoch 17: 100%|     | 10/10 [00:04<00:00,  2.48batch/s]
[Epoch 17]       training loss = -2.727  validation loss = -2.740
Epoch 18: 100%|     | 10/10 [00:04<00:00,  2.47batch/s]
[Epoch 18]       training loss = -2.728  validation loss = -2.741
Epoch 19: 100%|     | 10/10 [00:04<00:00,  2.46batch/s]
[Epoch 19]       training loss = -2.728  validation loss = -2.741
Epoch 20: 100%|     | 10/10 [00:04<00:00,  2.48batch/s]
[Epoch 20]       training loss = -2.729  validation loss = -2.742
Epoch 21: 100%|     | 10/10 [00:04<00:00,  2.46batch/s]
[Epoch 21]       training loss = -2.730  validation loss = -2.742
Epoch 22: 100%|     | 10/10 [00:04<00:00,  2.45batch/s]
[Epoch 22]       training loss = -2.730  validation loss = -2.742
Epoch 23: 100%|     | 10/10 [00:04<00:00,  2.44batch/s]
[Epoch 23]       training loss = -2.730  validation loss = -2.743
Epoch 24: 100%|     | 10/10 [00:04<00:00,  2.47batch/s]
[Epoch 24]       training loss = -2.730  validation loss = -2.743
Epoch 25: 100%|     | 10/10 [00:04<00:00,  2.46batch/s]
[Epoch 25]       training loss = -2.731  validation loss = -2.743
Epoch 26: 100%|     | 10/10 [00:04<00:00,  2.47batch/s]
[Epoch 26]       training loss = -2.730  validation loss = -2.743
Epoch 27: 100%|     | 10/10 [00:04<00:00,  2.46batch/s]
[Epoch 27]       training loss = -2.731  validation loss = -2.744
Epoch 28: 100%|     | 10/10 [00:04<00:00,  2.45batch/s]
[Epoch 28]       training loss = -2.730  validation loss = -2.744
Epoch 29: 100%|     | 10/10 [00:04<00:00,  2.44batch/s]
[Epoch 29]       training loss = -2.730  validation loss = -2.744
```

[23]:
```
fig, ax = plt.subplots()
ax.plot(np.arange(len(model_snrv.training_losses)), model_snrv.training_losses)
ax.plot(np.arange(len(model_snrv.validation_losses)), model_snrv.
  ↪validation_losses)
ax.set_xlabel('epoch')
```

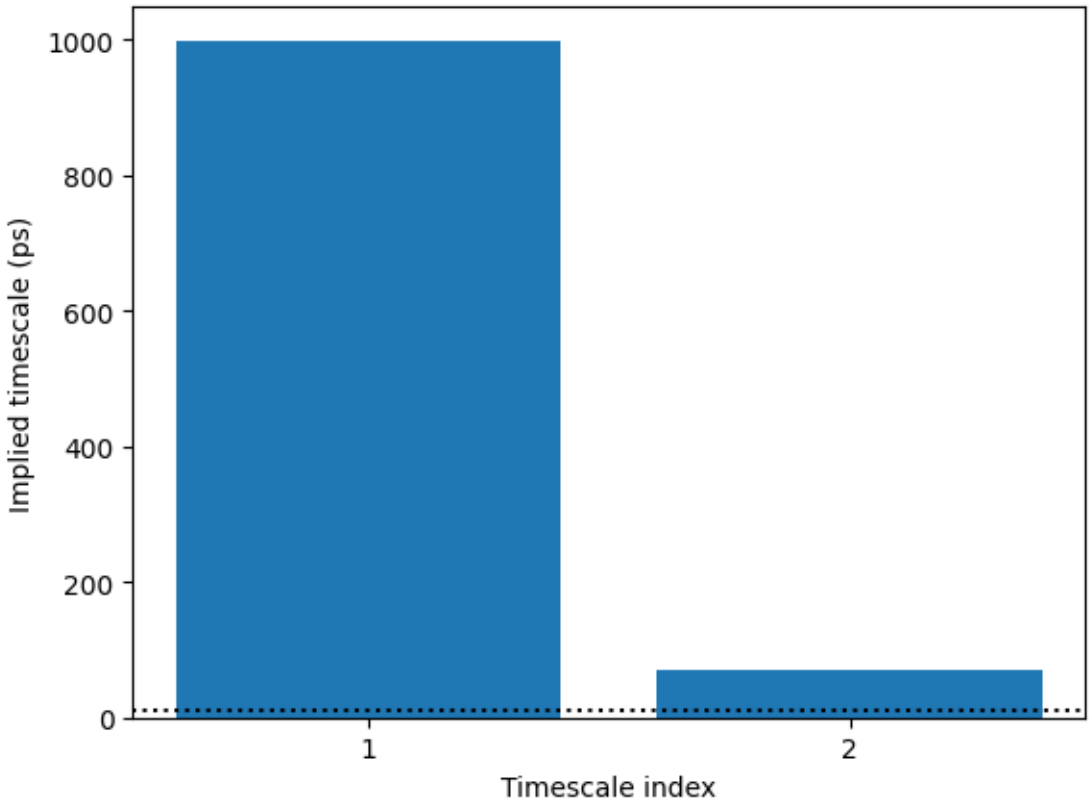
```
ax.set_ylabel('loss')
ax.legend(['training','validation'])
fig.tight_layout()
```



[24]:
```
save_freq = 1 # ps
```

[25]:
```
evals = model_snrv.evals.cpu().detach().numpy()
plt.bar(range(1,evals.size), -lag_n*save_freq/np.log(evals[1:]))
plt.ylabel('Implied timescale (ps)')
plt.xticks(range(1,evals.size))
plt.xlabel('Timescale index')
plt.axhline(lag_n*save_freq, color='k', linestyle=':')
```

[25]:
```
<matplotlib.lines.Line2D at 0x7b3245187370>
```



[26]:
```
model_snrv.eval()
```

[26]:
```
Snrv(
  (activation): GELU(approximate='none')
  (model): Sequential(
    (0): Linear(in_features=231, out_features=100, bias=True)
    (1): BatchNorm1d(100, eps=1e-05, momentum=0.1, affine=True,
track_running_stats=True)
    (2): GELU(approximate='none')
    (3): Linear(in_features=100, out_features=100, bias=True)
    (4): BatchNorm1d(100, eps=1e-05, momentum=0.1, affine=True,
track_running_stats=True)
    (5): GELU(approximate='none')
    (6): Linear(in_features=100, out_features=3, bias=True)
  )
)
```

[27]:
```
evecs = model_snrv.transform(torch.cat(coords_torch)).cpu().detach().numpy()
```

[28]:
```
trj_cat = md.join(trjs)
```

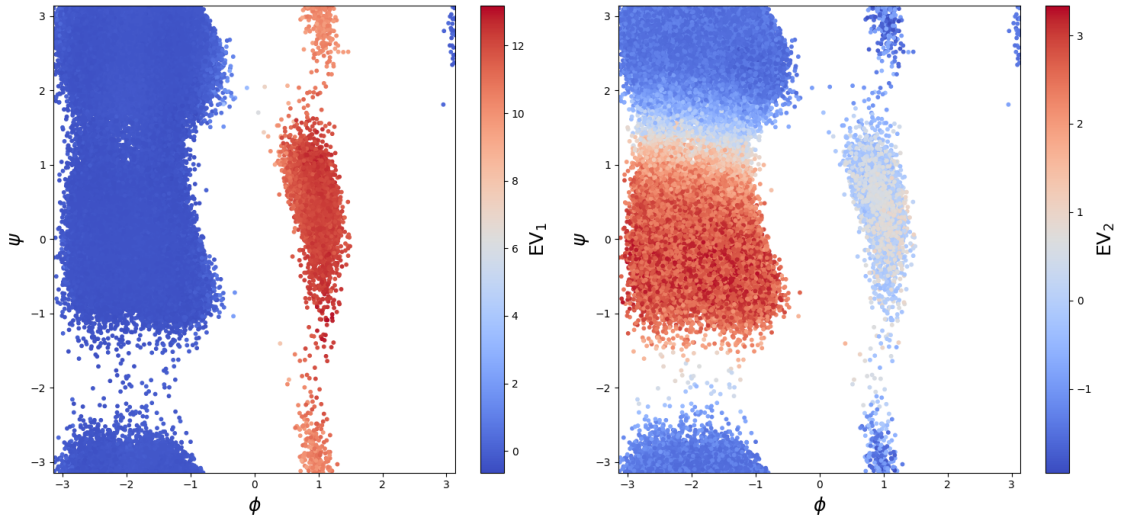
[29]:
```
phi = md.compute_phi(trj_cat)[1].flatten()
psi = md.compute_psi(trj_cat)[1].flatten()
```

[30]:
```
fig, axes = plt.subplots(1, 2, figsize = (15, 7))
axes = axes.flatten()

for e in range(1, evecs.shape[1]):
    evec = evecs[:, e]
    ax = axes[e-1]

    im = ax.scatter(phi, psi, c=evec, s=10, cmap='coolwarm')
    ax.set_xlabel('$\phi$', fontsize=18)
    ax.set_ylabel('$\psi$', fontsize=18)
    ax.set_xlim(-np.pi, np.pi)
    ax.set_ylim(-np.pi, np.pi)
    cbar = plt.colorbar(im, ax=ax)
    cbar.set_label(f'EV$_{e}$', size=18)

plt.tight_layout()
```



[31]:
```
CVs = [model_snrv.transform(x).cpu().detach()[:, 1:] for x in coords_torch]
CVs[0].shape, len(CVs)
```

[31]: (torch.Size([250000, 2]), 1)

5 MDN propagator (~3 mins)

[32]:
```
model_mdn = Propagator(dim = CVs[0].size(1))
```

[33]:
```
model_mdn.fit(CVs, lag = 10, max_epochs=10)
```

```
INFO:pytorch_lightning.utilities.rank_zero:GPU available: True (cuda), used:
True
INFO:pytorch_lightning.utilities.rank_zero:TPU available: False, using: 0 TPU
cores
INFO:pytorch_lightning.utilities.rank_zero:IPU available: False, using: 0 IPUs
INFO:pytorch_lightning.utilities.rank_zero:HPU available: False, using: 0 HPUs
INFO:pytorch_lightning.utilities.rank_zero:You are using a CUDA device ('NVIDIA
L4') that has Tensor Cores. To properly utilize them, you should set
`torch.set_float32_matmul_precision('medium' | 'high')` which will trade-off
precision for performance. For more details, read https://pytorch.org/docs/stabl
e/generated/torch.set_float32_matmul_precision.html#torch.set_float32_matmul_pre
cision
INFO:pytorch_lightning.accelerators.cuda:LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES:
[0]
INFO:pytorch_lightning.callbacks.model_summary:
  | Name    | Type                  | Params
-------------------------------------------------
0 | mdn     | MixtureDensityNetwork | 33.0 K
1 | _scaler | MinMaxScaler          | 0
-------------------------------------------------
33.0 K    Trainable params
0         Non-trainable params
33.0 K    Total params
0.132     Total estimated model params size (MB)
/usr/local/lib/python3.10/dist-
packages/pytorch_lightning/trainer/connectors/data_connector.py:441: The
'train_dataloader' does not have many workers which may be a bottleneck.
Consider increasing the value of the `num_workers` argument` to `num_workers=15`
in the `DataLoader` to improve performance.
```

```
Training: |          | 0/? [00:00<?, ?it/s]
```

```
INFO:pytorch_lightning.utilities.rank_zero:`Trainer.fit` stopped:
`max_epochs=10` reached.
```

[33]:
```
Propagator(
  (mdn): MixtureDensityNetwork(
    (network): MLP(
      (mlp): Sequential(
        (0): Linear(in_features=2, out_features=128, bias=True)
        (1): SiLU()
        (2): Linear(in_features=128, out_features=128, bias=True)
```

```
        (3): SiLU()
        (4): Linear(in_features=128, out_features=125, bias=True)
      )
    )
  )
  (_scaler): MinMaxScaler()
)
```

[34]:
```
n_steps = int(1E2)
x = CVs[0][0][None]
synthetic_traj_CVs = model_mdn.gen_synthetic_traj(x, n_steps)
```

```
  0%|          | 0/100 [00:00<?, ?it/s]
```

6 DDPM Decoder (~5 mins)

[35]:
```
xyz = list()
for trj in trjs:

    t_backbone = trj.atom_slice(trj.top.select('backbone')).center_coordinates()

    n = trj.xyz.shape[0]

    xyz.append(torch.tensor(t_backbone.xyz.reshape(n, -1)).float())
```

[36]:
```
model_ddpm = DDPM(xyz[0].shape[1], CVs[0].shape[1])
```

[37]:
```
model_ddpm.fit(xyz, CVs, max_epochs=3)
```

```
INFO:pytorch_lightning.utilities.rank_zero:GPU available: True (cuda), used:
True
INFO:pytorch_lightning.utilities.rank_zero:TPU available: False, using: 0 TPU
cores
INFO:pytorch_lightning.utilities.rank_zero:IPU available: False, using: 0 IPUs
INFO:pytorch_lightning.utilities.rank_zero:HPU available: False, using: 0 HPUs
/usr/local/lib/python3.10/dist-
packages/pytorch_lightning/callbacks/model_checkpoint.py:653: Checkpoint
directory /content/checkpoints exists and is not empty.
INFO:pytorch_lightning.accelerators.cuda:LOCAL_RANK: 0 - CUDA_VISIBLE_DEVICES:
[0]
INFO:pytorch_lightning.callbacks.model_summary:
  | Name              | Type              | Params
-------------------------------------------------------
0 | model             | GaussianDiffusion | 4.0 M
1 | ema_model         | GaussianDiffusion | 4.0 M
2 | _feature_scaler   | MinMaxScaler      | 0
```

```
3 | _condition_scaler | MinMaxScaler      | 0
-------------------------------------------------------
7.9 M     Trainable params
0         Non-trainable params
7.9 M     Total params
31.749    Total estimated model params size (MB)

Training: |          | 0/? [00:00<?, ?it/s]

INFO:pytorch_lightning.utilities.rank_zero:`Trainer.fit` stopped: `max_epochs=3`
reached.
```

[37]:
```
DDPM(
  (model): GaussianDiffusion(
    (denoise_fn): Unet1D(
      (init_conv): Conv1d(1, 32, kernel_size=(7,), stride=(1,), padding=(3,))
      (time_mlp): Sequential(
        (0): SinusoidalPosEmb()
        (1): Linear(in_features=32, out_features=128, bias=True)
        (2): GELU(approximate='none')
        (3): Linear(in_features=128, out_features=128, bias=True)
      )
      (downs): ModuleList(
        (0): ModuleList(
          (0-1): 2 x ResnetBlock(
            (mlp): Sequential(
              (0): SiLU()
              (1): Linear(in_features=128, out_features=64, bias=True)
            )
            (block1): Block(
              (proj): WeightStandardizedConv2d(32, 32, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 32, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (block2): Block(
              (proj): WeightStandardizedConv2d(32, 32, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 32, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (res_conv): Identity()
          )
          (2): Residual(
            (fn): PreNorm(
              (fn): LinearAttention(
                (to_qkv): Conv1d(32, 384, kernel_size=(1,), stride=(1,),
bias=False)
```

```
              (to_out): Sequential(
                (0): Conv1d(128, 32, kernel_size=(1,), stride=(1,))
                (1): LayerNorm()
              )
            )
            (norm): LayerNorm()
          )
        )
        (3): Conv1d(32, 32, kernel_size=(3,), stride=(2,), padding=(1,))
      )
      (1): ModuleList(
        (0-1): 2 x ResnetBlock(
          (mlp): Sequential(
            (0): SiLU()
            (1): Linear(in_features=128, out_features=64, bias=True)
          )
          (block1): Block(
            (proj): WeightStandardizedConv2d(32, 32, kernel_size=(3,),
stride=(1,), padding=(1,))
            (norm): GroupNorm(8, 32, eps=1e-05, affine=True)
            (act): SiLU()
          )
          (block2): Block(
            (proj): WeightStandardizedConv2d(32, 32, kernel_size=(3,),
stride=(1,), padding=(1,))
            (norm): GroupNorm(8, 32, eps=1e-05, affine=True)
            (act): SiLU()
          )
          (res_conv): Identity()
        )
        (2): Residual(
          (fn): PreNorm(
            (fn): LinearAttention(
              (to_qkv): Conv1d(32, 384, kernel_size=(1,), stride=(1,),
bias=False)
              (to_out): Sequential(
                (0): Conv1d(128, 32, kernel_size=(1,), stride=(1,))
                (1): LayerNorm()
              )
            )
            (norm): LayerNorm()
          )
        )
        (3): Conv1d(32, 64, kernel_size=(3,), stride=(2,), padding=(1,))
      )
      (2): ModuleList(
        (0-1): 2 x ResnetBlock(
```

```
            (mlp): Sequential(
              (0): SiLU()
              (1): Linear(in_features=128, out_features=128, bias=True)
            )
            (block1): Block(
              (proj): WeightStandardizedConv2d(64, 64, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 64, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (block2): Block(
              (proj): WeightStandardizedConv2d(64, 64, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 64, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (res_conv): Identity()
          )
          (2): Residual(
            (fn): PreNorm(
              (fn): LinearAttention(
                (to_qkv): Conv1d(64, 384, kernel_size=(1,), stride=(1,),
bias=False)
                (to_out): Sequential(
                  (0): Conv1d(128, 64, kernel_size=(1,), stride=(1,))
                  (1): LayerNorm()
                )
              )
              (norm): LayerNorm()
            )
          )
          (3): Conv1d(64, 128, kernel_size=(3,), stride=(2,), padding=(1,))
        )
        (3): ModuleList(
          (0-1): 2 x ResnetBlock(
            (mlp): Sequential(
              (0): SiLU()
              (1): Linear(in_features=128, out_features=256, bias=True)
            )
            (block1): Block(
              (proj): WeightStandardizedConv2d(128, 128, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 128, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (block2): Block(
              (proj): WeightStandardizedConv2d(128, 128, kernel_size=(3,),
```

```
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 128, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (res_conv): Identity()
          )
          (2): Residual(
            (fn): PreNorm(
              (fn): LinearAttention(
                (to_qkv): Conv1d(128, 384, kernel_size=(1,), stride=(1,),
bias=False)
                (to_out): Sequential(
                  (0): Conv1d(128, 128, kernel_size=(1,), stride=(1,))
                  (1): LayerNorm()
                )
              )
              (norm): LayerNorm()
            )
          )
          (3): Conv1d(128, 256, kernel_size=(3,), stride=(1,), padding=(1,))
        )
      )
      (ups): ModuleList(
        (0): ModuleList(
          (0-1): 2 x ResnetBlock(
            (mlp): Sequential(
              (0): SiLU()
              (1): Linear(in_features=128, out_features=512, bias=True)
            )
            (block1): Block(
              (proj): WeightStandardizedConv2d(384, 256, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 256, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (block2): Block(
              (proj): WeightStandardizedConv2d(256, 256, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 256, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (res_conv): Conv1d(384, 256, kernel_size=(1,), stride=(1,))
          )
          (2): Residual(
            (fn): PreNorm(
              (fn): LinearAttention(
                (to_qkv): Conv1d(256, 384, kernel_size=(1,), stride=(1,),
```

```
bias=False)
                (to_out): Sequential(
                  (0): Conv1d(128, 256, kernel_size=(1,), stride=(1,))
                  (1): LayerNorm()
                )
              )
              (norm): LayerNorm()
            )
          )
          (3): Sequential(
            (0): Upsample(scale_factor=2.0, mode='nearest')
            (1): Conv1d(256, 128, kernel_size=(3,), stride=(1,), padding=(1,))
          )
        )
        (1): ModuleList(
          (0-1): 2 x ResnetBlock(
            (mlp): Sequential(
              (0): SiLU()
              (1): Linear(in_features=128, out_features=256, bias=True)
            )
            (block1): Block(
              (proj): WeightStandardizedConv2d(192, 128, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 128, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (block2): Block(
              (proj): WeightStandardizedConv2d(128, 128, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 128, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (res_conv): Conv1d(192, 128, kernel_size=(1,), stride=(1,))
          )
          (2): Residual(
            (fn): PreNorm(
              (fn): LinearAttention(
                (to_qkv): Conv1d(128, 384, kernel_size=(1,), stride=(1,),
bias=False)
                (to_out): Sequential(
                  (0): Conv1d(128, 128, kernel_size=(1,), stride=(1,))
                  (1): LayerNorm()
                )
              )
              (norm): LayerNorm()
            )
          )
```

```
          (3): Sequential(
            (0): Upsample(scale_factor=2.0, mode='nearest')
            (1): Conv1d(128, 64, kernel_size=(3,), stride=(1,), padding=(1,))
          )
        )
        (2): ModuleList(
          (0-1): 2 x ResnetBlock(
            (mlp): Sequential(
              (0): SiLU()
              (1): Linear(in_features=128, out_features=128, bias=True)
            )
            (block1): Block(
              (proj): WeightStandardizedConv2d(96, 64, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 64, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (block2): Block(
              (proj): WeightStandardizedConv2d(64, 64, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 64, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (res_conv): Conv1d(96, 64, kernel_size=(1,), stride=(1,))
          )
          (2): Residual(
            (fn): PreNorm(
              (fn): LinearAttention(
                (to_qkv): Conv1d(64, 384, kernel_size=(1,), stride=(1,),
bias=False)
                (to_out): Sequential(
                  (0): Conv1d(128, 64, kernel_size=(1,), stride=(1,))
                  (1): LayerNorm()
                )
              )
              (norm): LayerNorm()
            )
          )
          (3): Sequential(
            (0): Upsample(scale_factor=2.0, mode='nearest')
            (1): Conv1d(64, 32, kernel_size=(3,), stride=(1,), padding=(1,))
          )
        )
        (3): ModuleList(
          (0-1): 2 x ResnetBlock(
            (mlp): Sequential(
              (0): SiLU()
```

```
              (1): Linear(in_features=128, out_features=64, bias=True)
            )
            (block1): Block(
              (proj): WeightStandardizedConv2d(64, 32, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 32, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (block2): Block(
              (proj): WeightStandardizedConv2d(32, 32, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 32, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (res_conv): Conv1d(64, 32, kernel_size=(1,), stride=(1,))
          )
          (2): Residual(
            (fn): PreNorm(
              (fn): LinearAttention(
                (to_qkv): Conv1d(32, 384, kernel_size=(1,), stride=(1,),
bias=False)
                (to_out): Sequential(
                  (0): Conv1d(128, 32, kernel_size=(1,), stride=(1,))
                  (1): LayerNorm()
                )
              )
              (norm): LayerNorm()
            )
          )
          (3): Conv1d(32, 32, kernel_size=(3,), stride=(1,), padding=(1,))
        )
      )
      (mid_block1): ResnetBlock(
        (mlp): Sequential(
          (0): SiLU()
          (1): Linear(in_features=128, out_features=512, bias=True)
        )
        (block1): Block(
          (proj): WeightStandardizedConv2d(256, 256, kernel_size=(3,),
stride=(1,), padding=(1,))
          (norm): GroupNorm(8, 256, eps=1e-05, affine=True)
          (act): SiLU()
        )
        (block2): Block(
          (proj): WeightStandardizedConv2d(256, 256, kernel_size=(3,),
stride=(1,), padding=(1,))
          (norm): GroupNorm(8, 256, eps=1e-05, affine=True)
```

```
          (act): SiLU()
        )
        (res_conv): Identity()
      )
      (mid_attn): Residual(
        (fn): PreNorm(
          (fn): Attention(
            (to_qkv): Conv1d(256, 384, kernel_size=(1,), stride=(1,),
bias=False)
            (to_out): Conv1d(128, 256, kernel_size=(1,), stride=(1,))
          )
          (norm): LayerNorm()
        )
      )
      (mid_block2): ResnetBlock(
        (mlp): Sequential(
          (0): SiLU()
          (1): Linear(in_features=128, out_features=512, bias=True)
        )
        (block1): Block(
          (proj): WeightStandardizedConv2d(256, 256, kernel_size=(3,),
stride=(1,), padding=(1,))
          (norm): GroupNorm(8, 256, eps=1e-05, affine=True)
          (act): SiLU()
        )
        (block2): Block(
          (proj): WeightStandardizedConv2d(256, 256, kernel_size=(3,),
stride=(1,), padding=(1,))
          (norm): GroupNorm(8, 256, eps=1e-05, affine=True)
          (act): SiLU()
        )
        (res_conv): Identity()
      )
      (final_res_block): ResnetBlock(
        (mlp): Sequential(
          (0): SiLU()
          (1): Linear(in_features=128, out_features=64, bias=True)
        )
        (block1): Block(
          (proj): WeightStandardizedConv2d(64, 32, kernel_size=(3,),
stride=(1,), padding=(1,))
          (norm): GroupNorm(8, 32, eps=1e-05, affine=True)
          (act): SiLU()
        )
        (block2): Block(
          (proj): WeightStandardizedConv2d(32, 32, kernel_size=(3,),
stride=(1,), padding=(1,))
```

```
          (norm): GroupNorm(8, 32, eps=1e-05, affine=True)
          (act): SiLU()
        )
        (res_conv): Conv1d(64, 32, kernel_size=(1,), stride=(1,))
      )
      (final_conv): Conv1d(32, 1, kernel_size=(1,), stride=(1,))
    )
  )
  (ema_model): GaussianDiffusion(
    (denoise_fn): Unet1D(
      (init_conv): Conv1d(1, 32, kernel_size=(7,), stride=(1,), padding=(3,))
      (time_mlp): Sequential(
        (0): SinusoidalPosEmb()
        (1): Linear(in_features=32, out_features=128, bias=True)
        (2): GELU(approximate='none')
        (3): Linear(in_features=128, out_features=128, bias=True)
      )
      (downs): ModuleList(
        (0): ModuleList(
          (0-1): 2 x ResnetBlock(
            (mlp): Sequential(
              (0): SiLU()
              (1): Linear(in_features=128, out_features=64, bias=True)
            )
            (block1): Block(
              (proj): WeightStandardizedConv2d(32, 32, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 32, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (block2): Block(
              (proj): WeightStandardizedConv2d(32, 32, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 32, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (res_conv): Identity()
          )
          (2): Residual(
            (fn): PreNorm(
              (fn): LinearAttention(
                (to_qkv): Conv1d(32, 384, kernel_size=(1,), stride=(1,),
bias=False)
                (to_out): Sequential(
                  (0): Conv1d(128, 32, kernel_size=(1,), stride=(1,))
                  (1): LayerNorm()
                )
```

```
              )
              (norm): LayerNorm()
            )
          )
          (3): Conv1d(32, 32, kernel_size=(3,), stride=(2,), padding=(1,))
        )
        (1): ModuleList(
          (0-1): 2 x ResnetBlock(
            (mlp): Sequential(
              (0): SiLU()
              (1): Linear(in_features=128, out_features=64, bias=True)
            )
            (block1): Block(
              (proj): WeightStandardizedConv2d(32, 32, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 32, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (block2): Block(
              (proj): WeightStandardizedConv2d(32, 32, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 32, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (res_conv): Identity()
          )
          (2): Residual(
            (fn): PreNorm(
              (fn): LinearAttention(
                (to_qkv): Conv1d(32, 384, kernel_size=(1,), stride=(1,),
bias=False)
                (to_out): Sequential(
                  (0): Conv1d(128, 32, kernel_size=(1,), stride=(1,))
                  (1): LayerNorm()
                )
              )
              (norm): LayerNorm()
            )
          )
          (3): Conv1d(32, 64, kernel_size=(3,), stride=(2,), padding=(1,))
        )
        (2): ModuleList(
          (0-1): 2 x ResnetBlock(
            (mlp): Sequential(
              (0): SiLU()
              (1): Linear(in_features=128, out_features=128, bias=True)
            )
```

```
            (block1): Block(
              (proj): WeightStandardizedConv2d(64, 64, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 64, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (block2): Block(
              (proj): WeightStandardizedConv2d(64, 64, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 64, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (res_conv): Identity()
          )
          (2): Residual(
            (fn): PreNorm(
              (fn): LinearAttention(
                (to_qkv): Conv1d(64, 384, kernel_size=(1,), stride=(1,),
bias=False)
                (to_out): Sequential(
                  (0): Conv1d(128, 64, kernel_size=(1,), stride=(1,))
                  (1): LayerNorm()
                )
              )
              (norm): LayerNorm()
            )
          )
          (3): Conv1d(64, 128, kernel_size=(3,), stride=(2,), padding=(1,))
        )
        (3): ModuleList(
          (0-1): 2 x ResnetBlock(
            (mlp): Sequential(
              (0): SiLU()
              (1): Linear(in_features=128, out_features=256, bias=True)
            )
            (block1): Block(
              (proj): WeightStandardizedConv2d(128, 128, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 128, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (block2): Block(
              (proj): WeightStandardizedConv2d(128, 128, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 128, eps=1e-05, affine=True)
              (act): SiLU()
            )
```

```
            (res_conv): Identity()
          )
          (2): Residual(
            (fn): PreNorm(
              (fn): LinearAttention(
                (to_qkv): Conv1d(128, 384, kernel_size=(1,), stride=(1,),
bias=False)
                (to_out): Sequential(
                  (0): Conv1d(128, 128, kernel_size=(1,), stride=(1,))
                  (1): LayerNorm()
                )
              )
              (norm): LayerNorm()
            )
          )
          (3): Conv1d(128, 256, kernel_size=(3,), stride=(1,), padding=(1,))
        )
      )
      (ups): ModuleList(
        (0): ModuleList(
          (0-1): 2 x ResnetBlock(
            (mlp): Sequential(
              (0): SiLU()
              (1): Linear(in_features=128, out_features=512, bias=True)
            )
            (block1): Block(
              (proj): WeightStandardizedConv2d(384, 256, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 256, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (block2): Block(
              (proj): WeightStandardizedConv2d(256, 256, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 256, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (res_conv): Conv1d(384, 256, kernel_size=(1,), stride=(1,))
          )
          (2): Residual(
            (fn): PreNorm(
              (fn): LinearAttention(
                (to_qkv): Conv1d(256, 384, kernel_size=(1,), stride=(1,),
bias=False)
                (to_out): Sequential(
                  (0): Conv1d(128, 256, kernel_size=(1,), stride=(1,))
                  (1): LayerNorm()
```

```
                )
              )
              (norm): LayerNorm()
            )
          )
          (3): Sequential(
            (0): Upsample(scale_factor=2.0, mode='nearest')
            (1): Conv1d(256, 128, kernel_size=(3,), stride=(1,), padding=(1,))
          )
        )
        (1): ModuleList(
          (0-1): 2 x ResnetBlock(
            (mlp): Sequential(
              (0): SiLU()
              (1): Linear(in_features=128, out_features=256, bias=True)
            )
            (block1): Block(
              (proj): WeightStandardizedConv2d(192, 128, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 128, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (block2): Block(
              (proj): WeightStandardizedConv2d(128, 128, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 128, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (res_conv): Conv1d(192, 128, kernel_size=(1,), stride=(1,))
          )
          (2): Residual(
            (fn): PreNorm(
              (fn): LinearAttention(
                (to_qkv): Conv1d(128, 384, kernel_size=(1,), stride=(1,),
bias=False)
                (to_out): Sequential(
                  (0): Conv1d(128, 128, kernel_size=(1,), stride=(1,))
                  (1): LayerNorm()
                )
              )
              (norm): LayerNorm()
            )
          )
          (3): Sequential(
            (0): Upsample(scale_factor=2.0, mode='nearest')
            (1): Conv1d(128, 64, kernel_size=(3,), stride=(1,), padding=(1,))
          )
```

```
        )
        (2): ModuleList(
          (0-1): 2 x ResnetBlock(
            (mlp): Sequential(
              (0): SiLU()
              (1): Linear(in_features=128, out_features=128, bias=True)
            )
            (block1): Block(
              (proj): WeightStandardizedConv2d(96, 64, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 64, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (block2): Block(
              (proj): WeightStandardizedConv2d(64, 64, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 64, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (res_conv): Conv1d(96, 64, kernel_size=(1,), stride=(1,))
          )
          (2): Residual(
            (fn): PreNorm(
              (fn): LinearAttention(
                (to_qkv): Conv1d(64, 384, kernel_size=(1,), stride=(1,),
bias=False)
                (to_out): Sequential(
                  (0): Conv1d(128, 64, kernel_size=(1,), stride=(1,))
                  (1): LayerNorm()
                )
              )
              (norm): LayerNorm()
            )
          )
          (3): Sequential(
            (0): Upsample(scale_factor=2.0, mode='nearest')
            (1): Conv1d(64, 32, kernel_size=(3,), stride=(1,), padding=(1,))
          )
        )
        (3): ModuleList(
          (0-1): 2 x ResnetBlock(
            (mlp): Sequential(
              (0): SiLU()
              (1): Linear(in_features=128, out_features=64, bias=True)
            )
            (block1): Block(
              (proj): WeightStandardizedConv2d(64, 32, kernel_size=(3,),
```

```
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 32, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (block2): Block(
              (proj): WeightStandardizedConv2d(32, 32, kernel_size=(3,),
stride=(1,), padding=(1,))
              (norm): GroupNorm(8, 32, eps=1e-05, affine=True)
              (act): SiLU()
            )
            (res_conv): Conv1d(64, 32, kernel_size=(1,), stride=(1,))
          )
          (2): Residual(
            (fn): PreNorm(
              (fn): LinearAttention(
                (to_qkv): Conv1d(32, 384, kernel_size=(1,), stride=(1,),
bias=False)
                (to_out): Sequential(
                  (0): Conv1d(128, 32, kernel_size=(1,), stride=(1,))
                  (1): LayerNorm()
                )
              )
              (norm): LayerNorm()
            )
          )
          (3): Conv1d(32, 32, kernel_size=(3,), stride=(1,), padding=(1,))
        )
      )
      (mid_block1): ResnetBlock(
        (mlp): Sequential(
          (0): SiLU()
          (1): Linear(in_features=128, out_features=512, bias=True)
        )
        (block1): Block(
          (proj): WeightStandardizedConv2d(256, 256, kernel_size=(3,),
stride=(1,), padding=(1,))
          (norm): GroupNorm(8, 256, eps=1e-05, affine=True)
          (act): SiLU()
        )
        (block2): Block(
          (proj): WeightStandardizedConv2d(256, 256, kernel_size=(3,),
stride=(1,), padding=(1,))
          (norm): GroupNorm(8, 256, eps=1e-05, affine=True)
          (act): SiLU()
        )
        (res_conv): Identity()
      )
```

```
      (mid_attn): Residual(
        (fn): PreNorm(
          (fn): Attention(
            (to_qkv): Conv1d(256, 384, kernel_size=(1,), stride=(1,),
bias=False)
            (to_out): Conv1d(128, 256, kernel_size=(1,), stride=(1,))
          )
          (norm): LayerNorm()
        )
      )
      (mid_block2): ResnetBlock(
        (mlp): Sequential(
          (0): SiLU()
          (1): Linear(in_features=128, out_features=512, bias=True)
        )
        (block1): Block(
          (proj): WeightStandardizedConv2d(256, 256, kernel_size=(3,),
stride=(1,), padding=(1,))
          (norm): GroupNorm(8, 256, eps=1e-05, affine=True)
          (act): SiLU()
        )
        (block2): Block(
          (proj): WeightStandardizedConv2d(256, 256, kernel_size=(3,),
stride=(1,), padding=(1,))
          (norm): GroupNorm(8, 256, eps=1e-05, affine=True)
          (act): SiLU()
        )
        (res_conv): Identity()
      )
      (final_res_block): ResnetBlock(
        (mlp): Sequential(
          (0): SiLU()
          (1): Linear(in_features=128, out_features=64, bias=True)
        )
        (block1): Block(
          (proj): WeightStandardizedConv2d(64, 32, kernel_size=(3,),
stride=(1,), padding=(1,))
          (norm): GroupNorm(8, 32, eps=1e-05, affine=True)
          (act): SiLU()
        )
        (block2): Block(
          (proj): WeightStandardizedConv2d(32, 32, kernel_size=(3,),
stride=(1,), padding=(1,))
          (norm): GroupNorm(8, 32, eps=1e-05, affine=True)
          (act): SiLU()
        )
        (res_conv): Conv1d(64, 32, kernel_size=(1,), stride=(1,))
```

```
      )
      (final_conv): Conv1d(32, 1, kernel_size=(1,), stride=(1,))
    )
  )
  (_feature_scaler): MinMaxScaler()
  (_condition_scaler): MinMaxScaler()
)
```

7 Decode synthetic traj (~2 mins)

[38]:
```
xyz_gen = model_ddpm.generate(synthetic_traj_CVs)
```

```
sampling loop time step:   0%|          | 0/1000 [00:00<?, ?it/s]
```

[39]:
```
xyz_gen = xyz_gen.reshape(xyz_gen.size(0), -1 , 3).numpy()
fake_trj = md.Trajectory(xyz = xyz_gen, topology=t_backbone.top)
fake_trj
```

[39]:
```
<mdtraj.Trajectory with 100 frames, 8 atoms, 3 residues, without unitcells at
0x7b32459e8190>
```

8 Visualize results (~1 min)

[40]:
```
v = nv.show_mdtraj(fake_trj)
v
```

```
NGLWidget(max_frame=99)
```

[41]:
```
fake_trj.save_pdb('ADP_backbone_synthetic_traj.pdb')
```