ADP_backbone_LSS

April 16, 2024

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

GitHub: 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} }

1.1 Allocating GPU accelerator (~1 min)

```
[2]: import torch
```

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

```
GPU available
```

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

```
[4]: 'cuda'
```

1.2 Install necessary packages (~10 mins)

```
[5]: %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 3.2 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
36.1 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
70.5 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
77.5 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-0.7.0-py3-none-any.whl (44 kB)
                          44.6/44.6 kB
5.7 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-2.2.2-py3-none-any.whl (801 kB)
                          801.9/801.9

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Collecting nglview
  Downloading nglview-3.1.2.tar.gz (5.5 MB)
                          5.5/5.5 MB
63.9 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

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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 16.0 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
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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 35.9 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) (1.4.0)
Requirement already satisfied: exceptiongroup>=1.0.0rc8 in /usr/local/lib/python3.10/dist-packages (from pytest) (1.2.0)
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
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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-

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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 55.5 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
32.7 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
35.2 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
59.9 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) (3.9.3)
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
78.5 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)
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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)
(0.1.6)
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
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/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
9.0 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 13.8 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 19.4 MB/s eta 0:00:00
Collecting qtpy>=2.4.0 (from qtconsole->jupyter)
  Downloading QtPy-2.4.1-py3-none-any.whl (93 kB)
                         93.5/93.5 kB
13.6 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) (3.6)
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=b68ec04600fbc79c33880bf79a494a948626a1d9afa67d47753d0ab182125e55
  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=7547276
sha256=7f1c262e344bbd0278e1f9a9a821c76914b402b2103fca47423862d95c6c9384
  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=2712147
sha256=16169bf1adc6b39af6d1ddc3eabf904155910404df38860fb2c59c9cb19e6e33
  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=cedeabf7c8335216a7b30f65452f1f7f8334c21965abe3b6ada16cc583d53532
  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=7644a3d588782a3b2f4584b331a35af02eeebed0112af295111ded5fc8b5eb43
  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-0.7.0
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-2.2.2 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-9yo46s3w
  Running command git clone --filter=blob:none --quiet
https://github.com/andrewlferguson/snrv.git /tmp/pip-req-build-9yo46s3w
  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=990400ad0de9544cda33596e8abf32c08ecef96cd5c0e3c07cf465c3917cd6d7
  Stored in directory: /tmp/pip-ephem-wheel-cache-
da38j82f/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-
jf_ayb75
  Running command git clone --filter=blob:none --quiet https://github.com/Ferg-
Lab/mdn_propagator.git /tmp/pip-req-build-jf_ayb75
  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=c8a5d4b997405ab7c7f1ca2cf6e316dbbe3e19c6f008780c821ce50ad19f14db
```

```
    Stored in directory: /tmp/pip-ephem-wheel-cache-
sywzyfsx/wheels/bc/a7/ff/4f2aa2dbe5dc942686e82380dbec7ba232e35df5f5213de831
Successfully built mdn_propagator
Installing collected packages: mdn_propagator
Successfully installed mdn_propagator-1.0.0+32.gad8fd32
```

[11]:
```python
%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-pvm3akdy
  Running command git clone --filter=blob:none --quiet https://github.com/Ferg-
Lab/molgen.git /tmp/pip-req-build-pvm3akdy
  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=e16936e84e8a03393df369cf6f1abac81068e5c876d8203487b057cb0879760c
  Stored in directory: /tmp/pip-ephem-wheel-cache-
cs5so774/wheels/1e/82/fb/a86e30e540a9156a4dfcf1eb19c92a23f5b728019e949672b1
Successfully built molgen
Installing collected packages: molgen
Successfully installed molgen-1.0.0+15.g533a1cc
```

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

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

1.3.1   Other dependencies

[13]:
```python
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()
```

2 Uploading files (~3 mins)

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

4 (ii) alanine-dipeptide-nowater.pdb

```
[15]: 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
Saving alanine-dipeptide-nowater.pdb to alanine-dipeptide-nowater.pdb

5 Load and prep data (~1 min)

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

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

```
[17]: [<mdtraj.Trajectory with 250000 frames, 22 atoms, 3 residues, and unitcells at
      0x7ef49d2f9690>]
```

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

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

```
[19]: 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
```

[19]: (1, torch.Size([250000, 231]))

6 SRV fitting (~5 mins)

[20]: ```
set_random_seed(42)
```

Setting random seed to 42

[21]: ```
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)
```

[22]: ```
lag_n = 10
```

[23]: ```
model_snrv.fit(coords_torch, lag=lag_n, scheduler=0.9)
```

Epoch 0: 100%| | 10/10 [00:05<00:00, 1.71batch/s]

[Epoch 0]   training loss = -2.017 validation loss = -2.289

Epoch 1: 100%| | 10/10 [00:05<00:00, 1.82batch/s]

[Epoch 1]   training loss = -2.415 validation loss = -2.408

```
Epoch 2: 100%|      | 10/10 [00:04<00:00,  2.32batch/s]

[Epoch 2]       training loss = -2.438  validation loss = -2.435

Epoch 3: 100%|      | 10/10 [00:05<00:00,  1.99batch/s]

[Epoch 3]       training loss = -2.450  validation loss = -2.448

Epoch 4: 100%|      | 10/10 [00:04<00:00,  2.32batch/s]

[Epoch 4]       training loss = -2.459  validation loss = -2.453

Epoch 5: 100%|      | 10/10 [00:04<00:00,  2.31batch/s]

[Epoch 5]       training loss = -2.472  validation loss = -2.473

Epoch 6: 100%|      | 10/10 [00:05<00:00,  1.99batch/s]

[Epoch 6]       training loss = -2.526  validation loss = -2.552

Epoch 7: 100%|      | 10/10 [00:04<00:00,  2.32batch/s]

[Epoch 7]       training loss = -2.632  validation loss = -2.618

Epoch 8: 100%|      | 10/10 [00:04<00:00,  2.04batch/s]

[Epoch 8]       training loss = -2.670  validation loss = -2.665

Epoch 9: 100%|      | 10/10 [00:04<00:00,  2.30batch/s]

[Epoch 9]       training loss = -2.694  validation loss = -2.659

Epoch 10: 100%|      | 10/10 [00:04<00:00,  2.35batch/s]

[Epoch 10]      training loss = -2.709  validation loss = -2.690

Epoch 11: 100%|      | 10/10 [00:04<00:00,  2.01batch/s]

[Epoch 11]      training loss = -2.716  validation loss = -2.712

Epoch 12: 100%|      | 10/10 [00:04<00:00,  2.27batch/s]

[Epoch 12]      training loss = -2.720  validation loss = -2.727

Epoch 13: 100%|      | 10/10 [00:04<00:00,  2.24batch/s]

[Epoch 13]      training loss = -2.723  validation loss = -2.731

Epoch 14: 100%|      | 10/10 [00:04<00:00,  2.13batch/s]

[Epoch 14]      training loss = -2.724  validation loss = -2.735

Epoch 15: 100%|      | 10/10 [00:04<00:00,  2.30batch/s]

[Epoch 15]      training loss = -2.726  validation loss = -2.738

Epoch 16: 100%|      | 10/10 [00:05<00:00,  1.78batch/s]

[Epoch 16]      training loss = -2.727  validation loss = -2.738

Epoch 17: 100%|      | 10/10 [00:07<00:00,  1.26batch/s]

[Epoch 17]      training loss = -2.727  validation loss = -2.740
```

```
Epoch 18: 100%|        | 10/10 [00:05<00:00,  1.99batch/s]

[Epoch 18]        training loss = -2.728  validation loss = -2.741

Epoch 19: 100%|        | 10/10 [00:04<00:00,  2.29batch/s]

[Epoch 19]        training loss = -2.728  validation loss = -2.741

Epoch 20: 100%|        | 10/10 [00:04<00:00,  2.02batch/s]

[Epoch 20]        training loss = -2.729  validation loss = -2.742

Epoch 21: 100%|        | 10/10 [00:04<00:00,  2.30batch/s]

[Epoch 21]        training loss = -2.730  validation loss = -2.742

Epoch 22: 100%|        | 10/10 [00:04<00:00,  2.28batch/s]

[Epoch 22]        training loss = -2.730  validation loss = -2.742

Epoch 23: 100%|        | 10/10 [00:05<00:00,  1.96batch/s]

[Epoch 23]        training loss = -2.730  validation loss = -2.743

Epoch 24: 100%|        | 10/10 [00:04<00:00,  2.29batch/s]

[Epoch 24]        training loss = -2.730  validation loss = -2.743

Epoch 25: 100%|        | 10/10 [00:05<00:00,  1.72batch/s]

[Epoch 25]        training loss = -2.731  validation loss = -2.743

Epoch 26: 100%|        | 10/10 [00:04<00:00,  2.27batch/s]

[Epoch 26]        training loss = -2.730  validation loss = -2.743

Epoch 27: 100%|        | 10/10 [00:04<00:00,  2.24batch/s]

[Epoch 27]        training loss = -2.731  validation loss = -2.744

Epoch 28: 100%|        | 10/10 [00:05<00:00,  1.97batch/s]

[Epoch 28]        training loss = -2.730  validation loss = -2.744

Epoch 29: 100%|        | 10/10 [00:04<00:00,  2.24batch/s]

[Epoch 29]        training loss = -2.730  validation loss = -2.744
```

```python
[24]: 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()
```
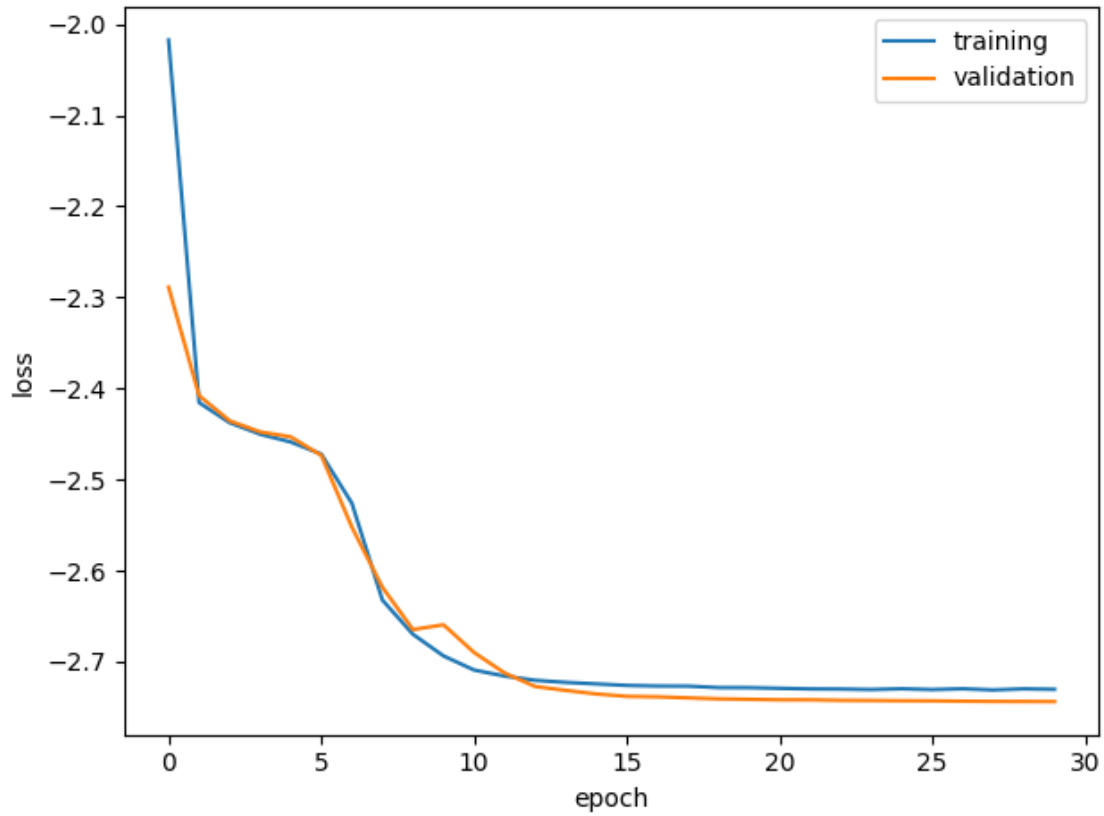
```
[25]: save_freq = 1 # ps
```
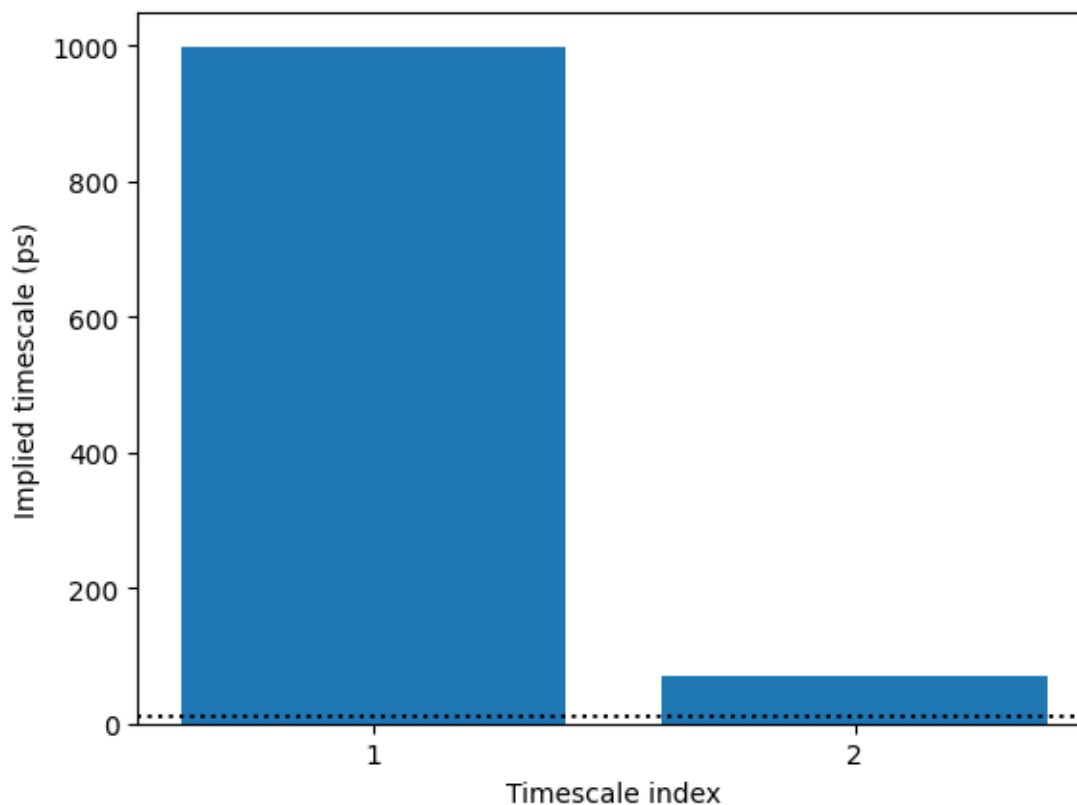
```
[26]: evals = model_snrv.evals.cpu().detach().numpy()
      plt.bar(range(1,evals.size), -lag_n*save_freq/np.log(evals[1:]))
      plt.ylabel('Implied timescale (ps)')
      plt.xticks(range(1,evals.size))
      plt.xlabel('Timescale index')
      plt.axhline(lag_n*save_freq, color='k', linestyle=':')
```

```
[26]: <matplotlib.lines.Line2D at 0x7ef5751eb490>
```

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

```
[27]: 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)
        )
      )
```

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

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

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

```
[31]: 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()
```
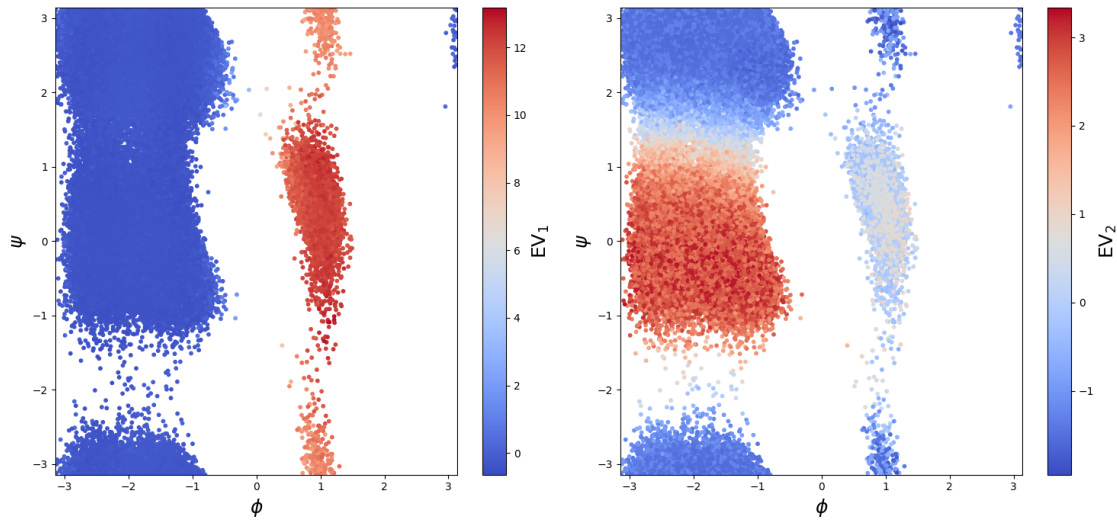


```
[32]: CVs = [model_snrv.transform(x).cpu().detach()[:, 1:] for x in coords_torch]
      CVs[0].shape, len(CVs)
```

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

20

7 MDN propagator (~3 mins)

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

```
[34]: 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.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)

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

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

```
[34]: 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()
      )
```

```
[35]: 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]
```

8   DDPM Decoder (~5 mins)

```
[43]: 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())
```

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

```
[45]: 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
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.
```

```
[45]: 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()
)
```

9   Decode synthetic traj (~2 mins)

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

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

```
[55]: 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
```

[55]: `<mdtraj.Trajectory with 100 frames, 8 atoms, 3 residues, without unitcells at 0x7ef43463ce80>`

10   Visualize results (~1 min)

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

`NGLWidget(max_frame=99)`

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