CS 726- Advanced ML

Assingment-1 Report

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We will be using Earth Movers Distance(emd) for all the further analysis of the performance of the model at various settings and conditions. We will consider the best value of "test_emd" of the three runs as the final metric value.

We used learnable time embedding by passing the time step(t) of x_t to a small 2-layer NN which generates a t_w = 16-dimension output, which We then concatenated with respective x_t to get an n_dim + t_w = 19-dimension input for each training example (x_t^i) after time embedding.

```
t_w = 16
self.time_embed = torch.nn.Sequential(torch.nn.Linear(1, 16),
                                      torch.nn.Tanh(),
                                      torch.nn.Linear(16, t_w),
                                      torch.nn.Tanh())
```

Fig. time embedding model used

1.Changing the Number of Training Steps:

Current model setting

- Model structure is:
  - w = 256

```
self.model = torch.nn.Sequential(
    torch.nn.Linear(t_w+3, w),
    torch.nn.Tanh(),
    torch.nn.Linear(w, 2*w),
    torch.nn.Tanh(),
    torch.nn.Linear(2*w, w),
    torch.nn.Tanh(),
    torch.nn.Linear(w, 3)
)
```

- Hyperparameters:
  - lbeta: 1.0e-05
  - n_dim: 3
  - n_steps: 50
  - ubeta: 0.0128
  - batch_size: 1024
  - learning_rate: 0.001

Number of Epochs = 500 (n_epochs=500)

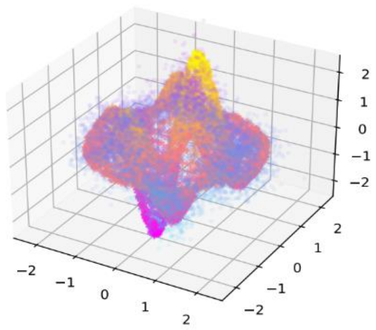
Results-

test_emd: 65.17553504955823

train_emd: 70.40486521231745

test_nll: 2.6779849529266357

train_nll: 2.670085906982422



Number of Epochs = 1000 (n_epochs=1000)

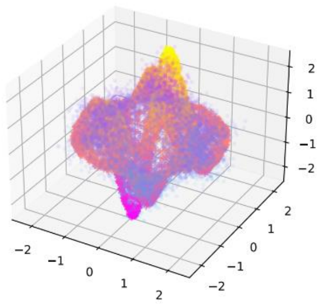
Results

test_emd: 66.36065731543384

train_emd: 66.31490655981473

test_nll: 2.6448776721954346

train_nll: 2.6374194622039795



Number of Epochs = 2000 (n_epochs=2000)

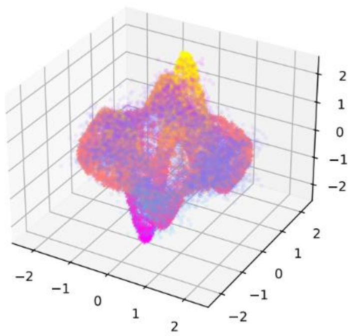
Results

test_emd: 63.07423301135008

train_emd: 62.0009674093369

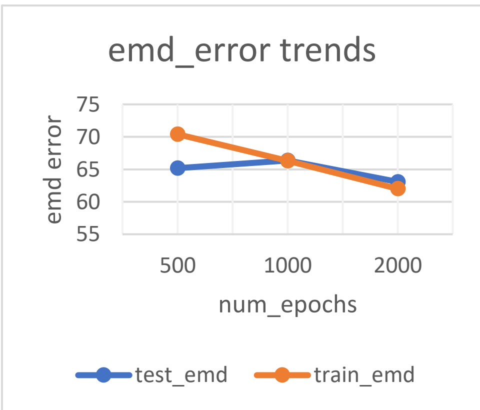
test_nll: 2.641606092453003

train_nll: 2.63297176361084



Analysis

- As the number of epochs increases there is very small change in test error, but it has decreased for large value so an indication that trying large value for num_epochs can be beneficial.
- train error decreases as num_epochs are increased it may be due to overfitting.
- So maybe we should some optimal number of epochs between 500-1000 and it would perform better because sample generated for higher num_epochs values are better as per visualisation.
- So, lets choose 600 as optimal value for n_epoch.



2. Model complexity:

Current model setting

- W = 256
- Hyperparameters:
    - lbeta: 1.0e-05
    - n_dim: 3
    - n_steps: 50
    - ubeta: 0.0128
    - batch_size: 1024
    - learning_rate: 0.001
    - n_epochs: 600

Simple Model, 72K trainable parameters

```
self.model = torch.nn.Sequential(
    torch.nn.Linear(t_w+3, w),
    torch.nn.Tanh(),
    torch.nn.Linear(w, w),
    torch.nn.Tanh(),
    torch.nn.Linear(w, 3)
)
```

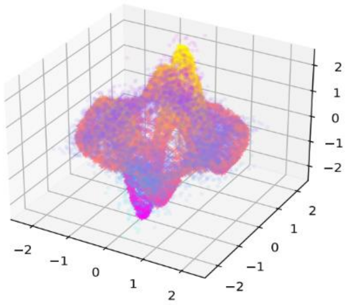
Results

test_emd: 63.30597077579907

train_emd: 64.55693641071107

test_nll: 2.654146671295166

train_nll: 2.6470699310302734



Complex Model, 1.3M trainable parameters

```
self.model = torch.nn.Sequential(
    torch.nn.Linear(t_w+3, w),
    torch.nn.Tanh(),
    torch.nn.Linear(w, 2*w),
    torch.nn.Tanh(),
    torch.nn.Linear(2*w, 4*w),#
    torch.nn.Tanh(),#
    torch.nn.Linear(4*w, 2*w),#
    torch.nn.Tanh(),#
    torch.nn.Linear(2*w, w),
    torch.nn.Tanh(),
    torch.nn.Linear(w, 3)
)
```

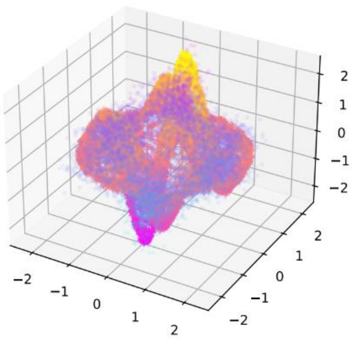
Results

test_emd: 70.31164168610466

train_emd: 62.754993318713986

test_nll: 2.6775283813476562

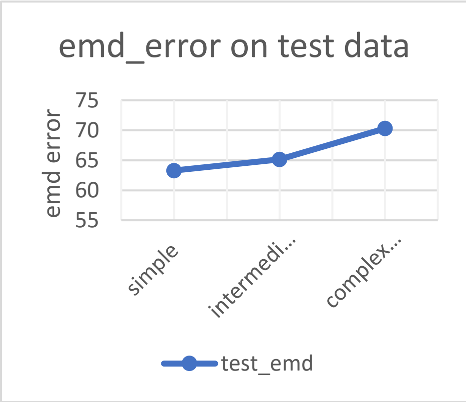
train_nll: 2.6704649925231934



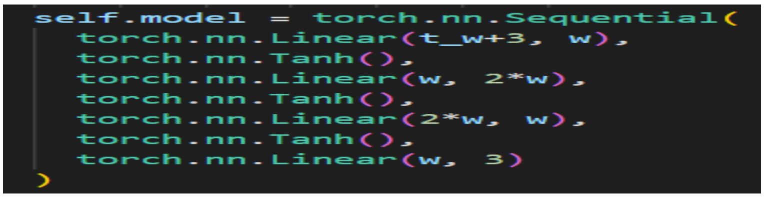
NOTE: the third intermediate model is same as we trained on previous part of the assingment, and the number of epochs are similar so have not trained it again

Analysis

- As the model gets complex training time increases.
- training error has increased for very complex model.
- It seems that a very simple model works fine for this toy dataset.
- We will choose an intermediate model, the model in which we did number of epoch testing because it seems like a good model with enough parameters and optimal training time and memory requirements.



So, our final model is – (w=256)



And num_epochs = 600

3. Number of diffusion steps (T):

For 3d_sin_5_5 data

Current model setting

- W = 256
- Hyperparameters:
  - lbeta: 1.0e-05
  - n_dim: 3
  - ubeta: 0.0128
  - batch_size: 1024
  - learning_rate: 0.001
  - n_epochs: 600
  - dataset used = 3d_sin_5_5 data

Number of Steps = 10, n_steps = 10

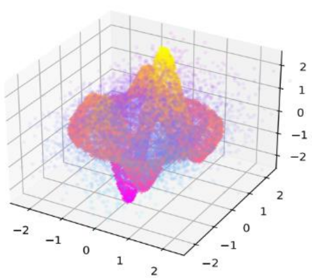
Results

test_emd: 83.30035817586062

train_emd: 81.41897810190828

test_nll: 2.9109654426574707

train_nll: 2.8995320796966553



Number of Steps = 50, n_steps = 50

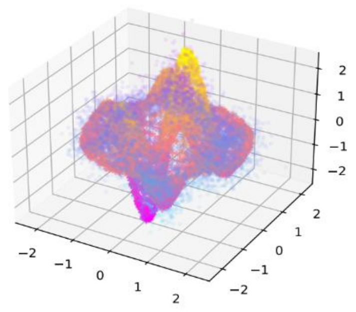
Results-

test_emd: 65.17553504955823

train_emd: 70.40486521231745

test_nll: 2.6779849529266357

train_nll: 2.670085906982422



Number of Steps = 100, n_steps = 100

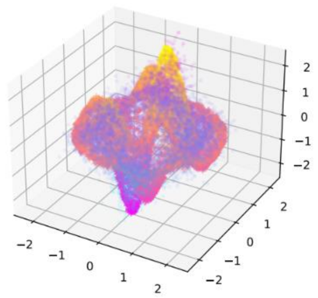
Results

test_emd: 62.59729977226936

train_emd: 64.6123901338262

test_nll: 2.6689274311065674

train_nll: 2.6577916145324707



Number of Steps = 150, n_steps = 150

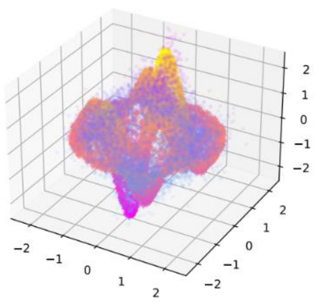
Results

test_emd: 64.7138290425177

train_emd: 66.87266873899209

test_nll: 2.6902542114257812

train_nll: 2.6812427043914795



Number of Steps = 200, n_steps = 200

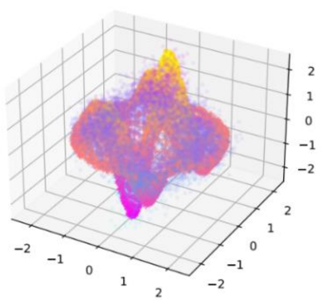
Results

test_emd: 69.04824575353155

train_emd: 69.0003225412479

test_nll: 2.680298089981079

train_nll: 2.670194387435913



for helix_3D data

Current model setting

- W = 256
- Hyperparameters:
    - lbeta: 1.0e-05
    - n_dim: 3

- ubeta: 0.0128
- batch_size: 1024
- learning_rate: 0.001
- n_epochs: 600

Number of Steps = 10, n_steps = 10

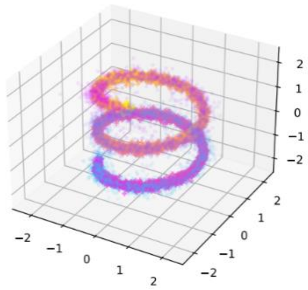
Results

test_emd: 58.99251491490972

train_emd: 48.61157009063477

test_nll: 2.352220058441162

train_nll: 2.346301317214966



Number of Steps = 50, n_steps = 50

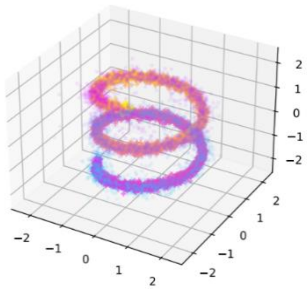
Results

test_emd: 51.35311040806201

train_emd: 70.57267437383348

test_nll: 2.3485875129699707

train_nll: 2.3438773155212402



Number of Steps = 100, n_steps = 100

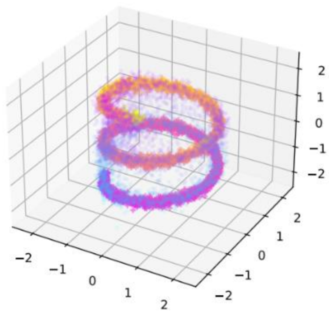
Results

test_emd: 51.60572010533156

train_emd: 50.26444759378028

test_nll: 2.3474135398864746

train_nll: 2.3469741344451904



Number of Steps = 150, n_steps = 150

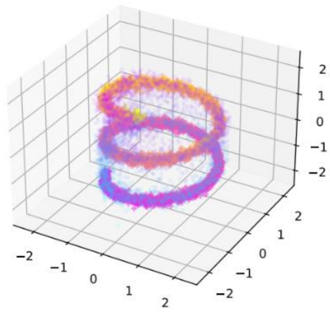
Results

test_emd: 53.12005686204001

train_emd: 63.921479221190125

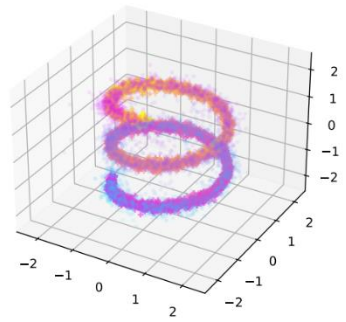
test_nll: 2.3685905933380127

train_nll: 2.3659677505493164



Number of Steps = 200, n_steps = 200

Results



test_emd: 46.17424568125869

train_emd: 50.38415121867081

test_nll: 2.3596997261047363

train_nll: 2.357518196105957

Analysis

- Here we have mentioned the best results out of the three evaluation, for all the different case.
- By overlooking at the data we can infer that by increasing the steps (T) we can get better results i.e., smaller value for EMD
- We can observe that after 100 steps the change in EMD is not significance

4. Number of diffusion steps (T):

For 3d_sin_5_5 data

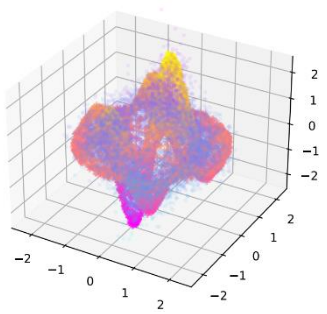
Current model setting

- W = 256
- Hyperparameters:
    - lbeta: 1.0e-05
    - n_dim: 3
    - n_steps: 150
    - ubeta: 0.0128
    - batch_size: 1024
    - learning_rate: 0.001
    - n_epochs: 600

"Linear" Noise schedule

Beta values are linearly varying with t

Results



test_emd: 68.95116409595362

train_emd: 71.0804771180983

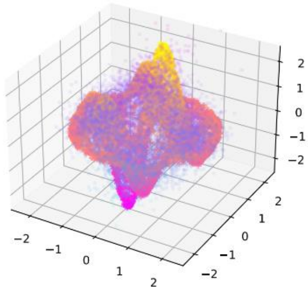
test_nll: 2.6895651817321777

train_nll: 2.680345058441162

“Constant” Noise schedule

Beta values are equal to ubeta value for all t.

Results



test_emd: 63.72570935469814

train_emd: 74.0343293062074

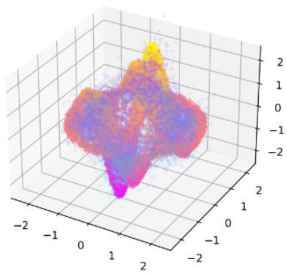
test_nll: 2.7506325244903564

train_nll: 2.739440679550171

“Quadratic” Noise schedule

Beta values are following a quadratic function over t and range is [lbeta, ubeta].

Results



test_emd: 67.027948243499

train_emd: 70.11542925460446

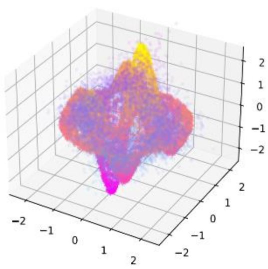
test_nll: 2.677572250366211

train_nll: 2.668335437774658

“warmup10” Noise schedule

Beta values ranges linearly from [lbeta to ubeta] in first 10% of total timesteps and later all values of betas are equal to ubeta. {on graph- linear function followed by const. value function}

Results



test_emd: 71.02178100826868

train_emd: 86.69617083708691

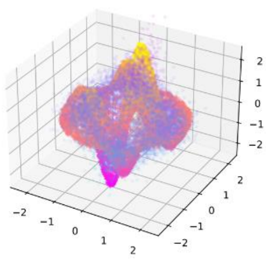
test_nll: 2.724071979522705

train_nll: 2.7135508060455322

“warmup50” Noise schedule

Beta values ranges linearly from [lbeta to ubeta] in first 50% of total timesteps and later all values of betas are equal to ubeta. {on graph- linear function followed by const. value function}

Results



test_emd: 66.07125496063745

train_emd: 76.25061033049296

test_nll: 2.7245938777923584

train_nll: 2.7167930603027344

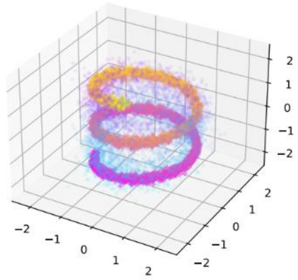
For helix_3D data

Current model setting

- W = 256
- Hyperparameters:
  - lbeta: 1.0e-05
  - n_dim: 3
  - n_steps: 150
  - ubeta: 0.0128
  - batch_size: 1024
  - learning_rate: 0.001
  - n_epochs: 600

"Linear" Noise schedule

Results



test_emd: 59.00353418889661

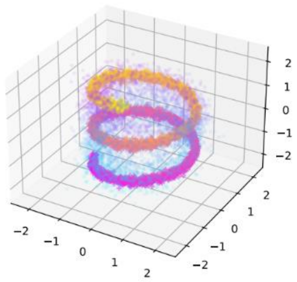
train_emd: 74.9186193992157

test_nll: 2.3739233016967773

train_nll: 2.370929002761841

"Constant" Noise schedule

Results



test_emd: 70.05747486392498

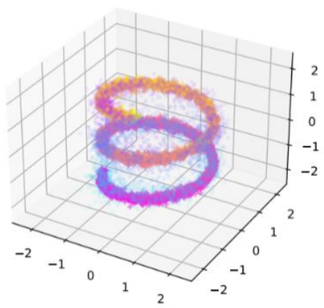
train_emd: 64.9508319559166

test_nll: 2.646155595779419

train_nll: 2.644508123397827

"Quadratic" Noise schedule

Results



test_emd: 59.34619851891867

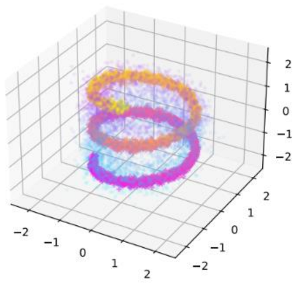
train_emd: 61.26329202036436

test_nll: 2.3793678283691406

train_nll: 2.3778738975524902

"warmup10" Noise schedule

Results



test_emd: 69.262612540213

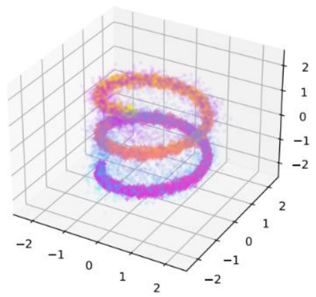
train_emd: 64.53478288896034

test_nll: 2.568970203399658

train_nll: 2.5658304691314697

“warmup50” Noise schedule

Results



test_emd: 63.84509899787168

train_emd: 63.27920885475712

test_nll: 2.4459991455078125

train_nll: 2.4439995288848877

Analysis

- In both dataset the linear scheduling seems to work fine.
- Constant noise factor destroys the information very quickly, and seems to not work very well.
- The warmup50 noise scheduling also works fine and in 3d_sin_5_5 data its produces better result.

Final Results/Conclusion

- Our final model is-

```
self.model = torch.nn.Sequential(
    torch.nn.Linear(t_w+3, w),
    torch.nn.Tanh(),
    torch.nn.Linear(w, 2*w),
    torch.nn.Tanh(),
    torch.nn.Linear(2*w, w),
    torch.nn.Tanh(),
    torch.nn.Linear(w, 3)
)
```

- Optimal number of epochs – 600
- Number of Steps(T) = 150
- Optimal Noise Scheduler = Linear and warmup50

--- Thank You ---