# Machine Learning for Solving PDEs HW3

In [1]:
```
import numpy as np
import torch
import torch.nn as nn
import torch.nn.functional as F
from math import sqrt
import gc
```

In [2]:
```
import torch
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
```

## Notes

Under the settings of discrete diffusion, the states at each sites transition sporadically, in the sense that under continuous time modeling, the probability of a state transitioning into a different one undergoes exponential distribution in $t$ before reaching a new state. This poses a different kind of challenge when simulating the process, but also provides unique advantages due to the state space $\chi$ on each site being discrete.

The paper *Score-based continuous-time discrete diffusion models* by Sun et al. introduced two reverse sampling processes, first by a discrete time sampling simulated using Eulerian steps, which requires a marginal distribution $p_t(X_t^d|x_t^{\textbackslash d};\theta)$ to be learned, while the second utilizes an analytical sampling technique which learns a bridging marginal distribution on $p_{0|t}(x_0^d|x_t^{\textbackslash d};\theta)$.

In our case we will learn the local marginal distribution $p_t(X_t^d|x_t^{\textbackslash d};\theta)$, due to its backward sampling more closely resembling a natural diffusion process, and potentially lessened dependence on intial sample size.

## Setup

In [3]:
```
import torch

# Compute Ising Potential

def V_batch(x, J=1.0):
    """
    x: Tensor of shape (B, N), with values in {-1, +1}
    Returns: Tensor of shape (B,), energy of each sample
    """
    # Circularly shift x by -1 to get neighbors
    x_shifted = torch.roll(x, shifts=-1, dims=1)
    energy = -J * torch.sum(x * x_shifted, dim=1)
    return energy
```

We simulate the process with Glauber dynamics:

1. Pick a site at random
2. $p(x_i=a|x_{-i}) \propto e^{-\Delta V(x)/T}$

In [4]:
```
import torch

def glauber_sampler(x, energy_fn, itr = 10000, T=1.0):
    """
    Glauber dynamics sampler for discrete Ising model
    x: [B, N] tensor of spins in {-1, +1}, modified in-place
    energy_fn: function that takes [B, N] tensor and returns [B] energies
    steps: number of update steps
    T: temperature
    """
    B, N = x.shape
    for _ in range(itr):
        # Randomly choose spin indices to update for each sample
        flip_indices = torch.randint(0, N, (B,), device=x.device)

        # Compute energy difference
        E_old = energy_fn(x)

        # Propose flipping one spin per batch item
        x[torch.arange(B), flip_indices] *= -1

        E_new = energy_fn(x)
        dE = E_new - E_old

        # Compute flip probabilities using Metropolis rule
        prob = torch.sigmoid(-dE / T)  # equivalent to min(1, exp(-dE/T))

        # Accept/reject proposals
        reject = torch.rand(B, device=x.device) >= prob
        x[torch.arange(B)[reject], flip_indices[reject]] *= -1

    return x
```

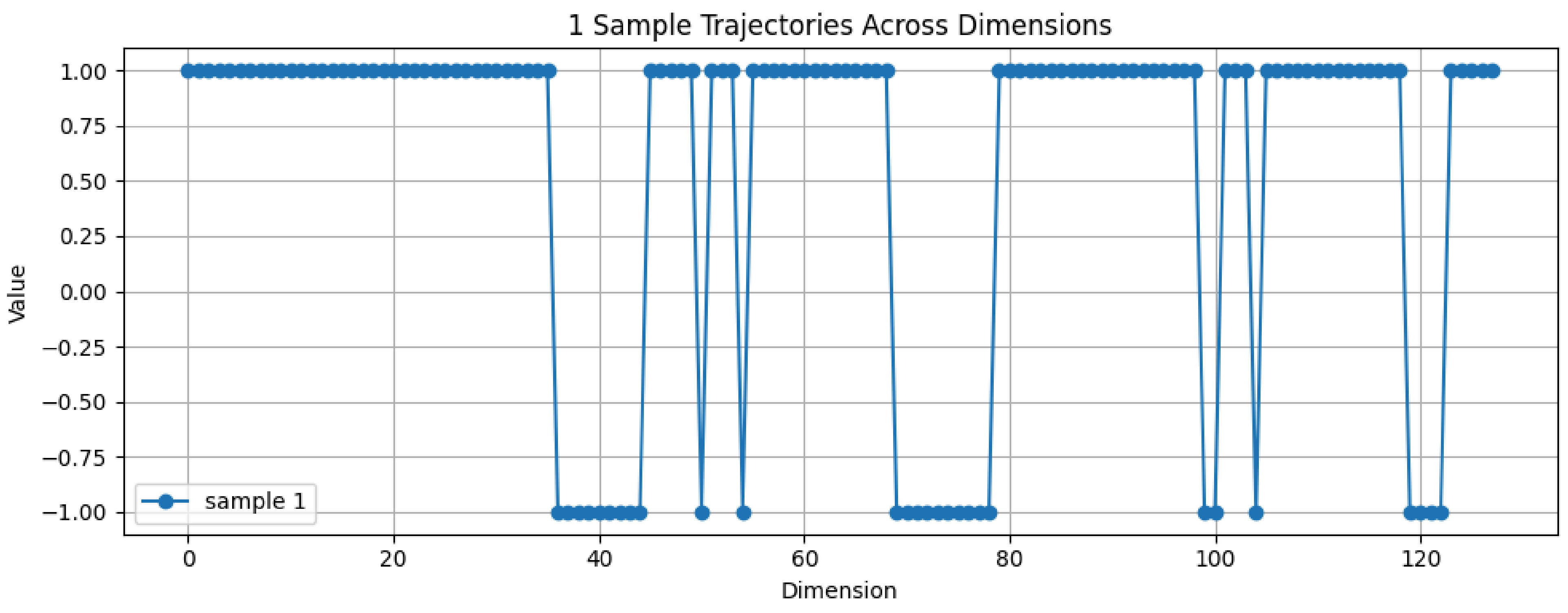
In [5]:
```
# samples N langevin based samples of dimension d
def sample(N, d, T = 1):
    # Config
    L = 2.5             # domain range
    itr = 100*d         # number of Langevin steps, needs to grow linearly with dimension
    h = 3e-4            # step size

    # Initialize from Uniform[-L, L]^d
    x0 = torch.randint(0, 2, (N, d)) * 2 -1  # shape [B, d]

    # Run simulation
    x_final = glauber_sampler(x0, V_batch, itr=itr, T=T)
    return x_final
```

In [6]:
```
X0 = sample(100, 128)
X0.shape
```

Out[6]:
```
torch.Size([100, 128])
```

In [7]:
```
import matplotlib.pyplot as plt
import numpy as np

def visualize_sample(x_np, num_samples=3):
    """
    Visualize a few samples as horizontal line plots across dimensions.

    x_np: [N, D] numpy array
    num_samples: how many samples to show
    """
    D = x_np.shape[1]
    sample_indices = np.random.choice(len(x_np), size=num_samples, replace=False)
    samples = x_np[sample_indices]

    plt.figure(figsize=(10, 4))
    for i, sample in enumerate(samples):
        plt.plot(range(D), sample, marker='o', label=f"sample {i+1}")

    plt.xlabel("Dimension")
    plt.ylabel("Value")
    plt.title(f"{num_samples} Sample Trajectories Across Dimensions")
    plt.legend()
    plt.grid(True)
    plt.tight_layout()
    plt.show()
```

In [8]:
```
visualize_sample(X0, 1)
```



## Discrete Diffusion training

### Forward Sampling

We have the following forward diffusion process:

$$\frac{d}{dt} q_{t|s}(x_t|x_s) = \sum_{x\in\chi} q_{t|s}(x|x_s) Q_t(x, x_t),$$

where $Q_t = Q\beta(t)$ is the transition matrix.

Here, we use the uniform stationary base rate, with $n$ the dimension of the sites,

$$Q = \mathbf{1}\mathbf{1}^T - n\mathbb{I} \equiv P\Lambda P^{-1},$$

which can be thought of as a tendency toward a uniform distribution.

We can further check that Q satisfies the l1 preservation rule, namely $\forall q \in \mathbb{R}^n, ||q||_1 = 1, ||Qq||_1 = 0$.

Explicitly, subtransition matrix in each dimension can be computed as

$$q^d_{t|s} = \left[ P \exp\left( \Lambda \int_s^t \beta(\tau) d\tau \right) P^{-1} \right]_d .$$

We let $\beta(\tau)$ be constantly 1, so that $\int_s^t \beta(\tau)d\tau$ is simply $t - s$, and the distribution should become fully uniform at $T = 1$

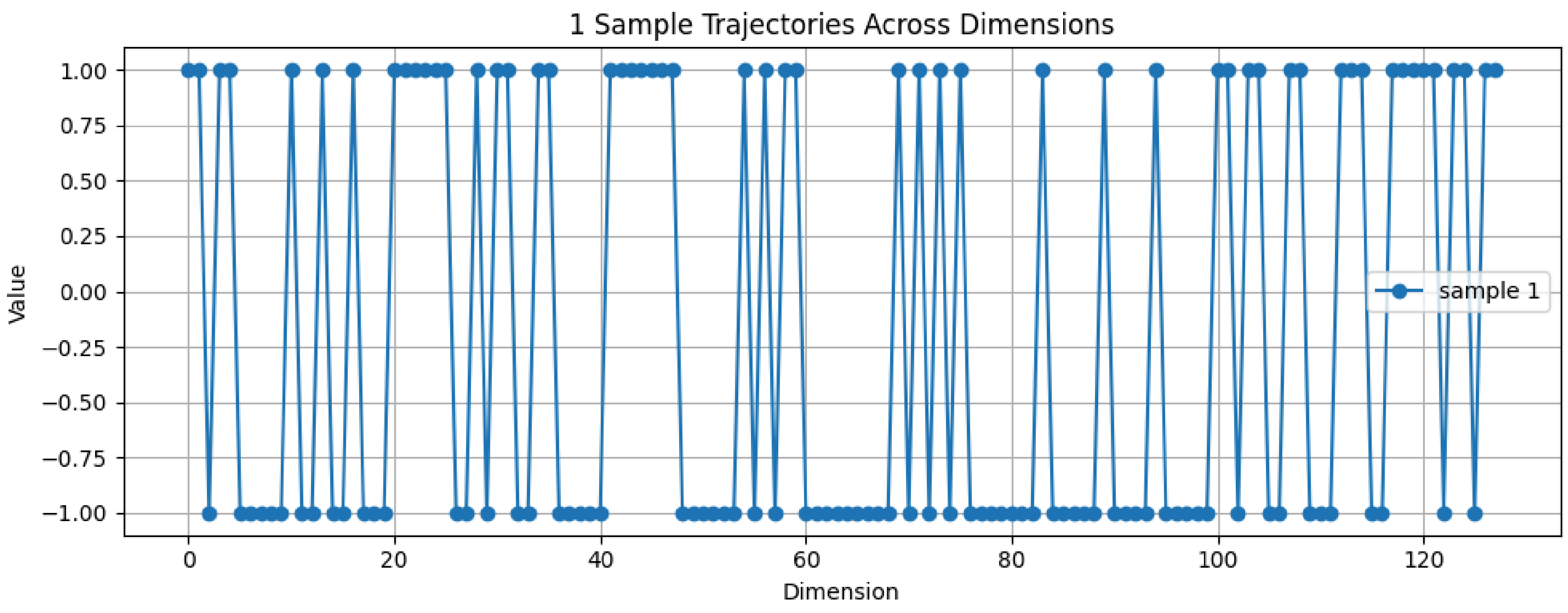
In [9]:
```
def diagonalize_Q(d):
    # Step 1: Construct Q in NumPy
    one = np.ones((d, 1))
    Q_np = (one @ one.T) - d*np.eye(d)

    # Step 2: Eigen-decomposition (since Q is symmetric, use eigh)
    eigvals, eigvecs = np.linalg.eigh(Q_np)  # eigvecs @ diag(eigvals) @ eigvecs.T = Q_np

    # Step 3: Convert to PyTorch tensors
    Q = torch.tensor(Q_np, dtype=torch.float64)
    P = torch.tensor(eigvecs, dtype=torch.float64)

    return Q, P, eigvals

def transition(h, P, eigvals):
    return P@torch.diag(torch.tensor(np.exp(eigvals*h)))@(P.T)
```

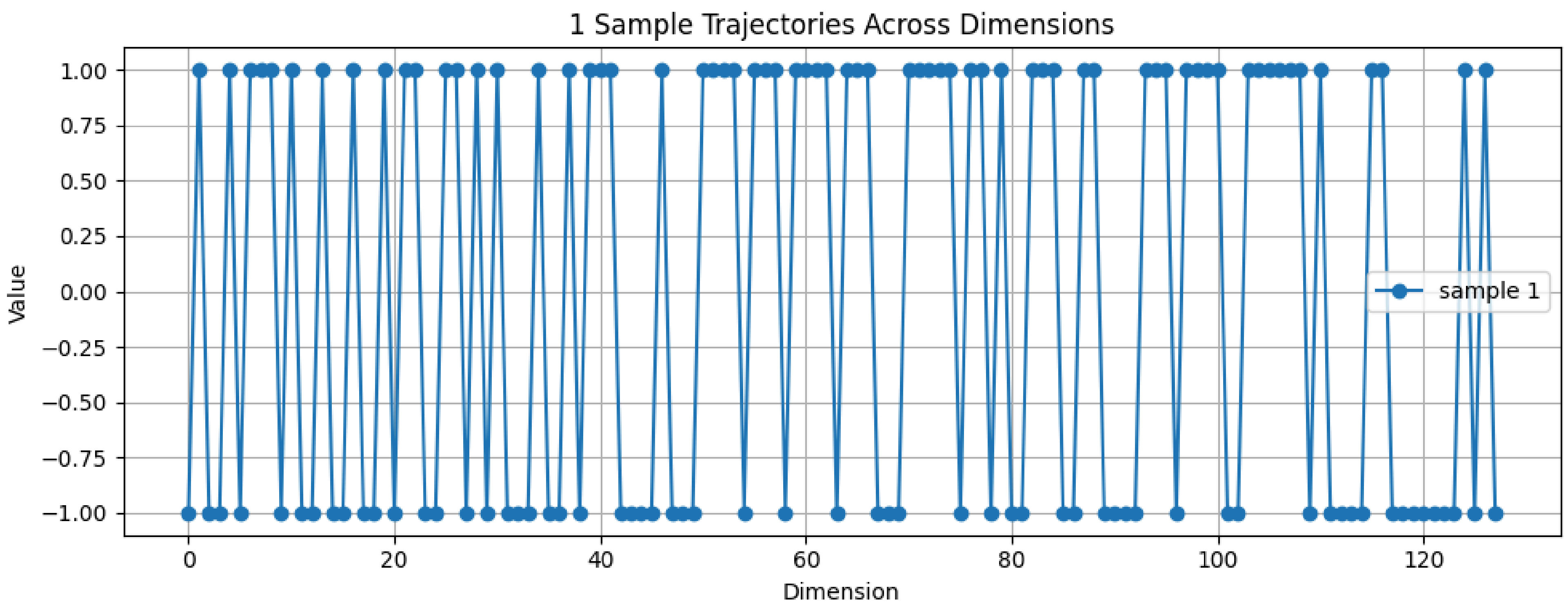
In [10]:
```
Q, P, eigvals =  diagonalize_Q(2)
# P@ Lambda @P.T
transition(0.01, P, eigvals)[:, 0]
```

Out[10]:
```
tensor([0.9901, 0.0099], dtype=torch.float64)
```

In [11]:
```
# diffusion based sampler
def forward_sampler(t1, h, X0, viz=False):
    d = X0.shape[1]
    N = X0.shape[0]
    buffer = []
    ts = []
    # without disturbing the original samples
    X = X0.clone()
    buffer.append(X)
    ts.append(t1)
    # compute a static transition matrix
    Q, P, eigvals =  diagonalize_Q(2)
    tr = transition(h, P, eigvals)
    # for dimension = 2 this degenerates
    # into a single bit flip probability p
    p = tr[0,1]
    while(t1>0):
        t1-=h
        accept = torch.rand((N,d), device=X.device) < p
        X[accept]*=-1
        if(viz and t1//h%500 == 0):
            visualize_sample(X, 1)
        buffer.append(X.clone())
        ts.append(t1)
    return torch.stack(buffer), torch.tensor(ts)

def flatten(layers, ts):
    """
    layers: Tensor of shape (T, N, d)
    ts: Tensor of shape (T,) - time values
    Returns: Tensor of shape (T*N, d+1)
    """
    T, N, d = layers.shape

    # Repeat time values for each sample in a layer
    time_column = ts[:, None].expand(T, N).reshape(-1, 1)  # shape (T*N, 1)
    # Flatten the layer data
    x_flat = layers.reshape(-1, d)  # shape (T*N, d)
    # Concatenate time as the last dimension
    concatenated = torch.cat([x_flat, time_column], dim=1)
    # we take the 1st to last of the time labeled data as x
    # we take the 0th to last-1th of original data as y
    # so that each input maps to the output which is the previous layer's samples
    return concatenated # shape (T*N, d+1)
```

In [12]:
```
forward_sampler(1, 0.001,X0,True)
```





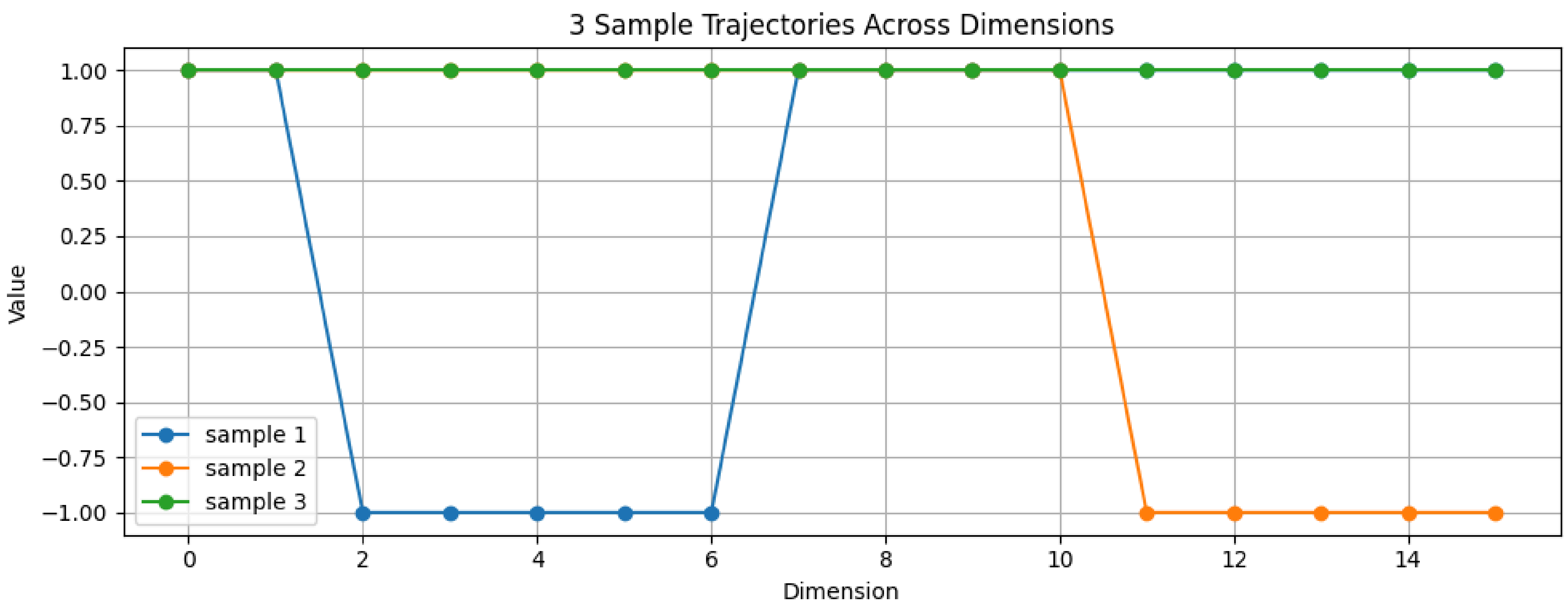
```
Out[12]: (tensor([[[-1,  1,  1,  ...,  1, -1, -1],
          [ 1,  1,  1,  ...,  1, -1, -1],
          [-1, -1,  1,  ...,  1, -1,  1],
          ...,
          [ 1,  1,  1,  ..., -1,  1,  1],
          [-1,  1,  1,  ...,  1, -1, -1],
          [-1, -1, -1,  ...,  1, -1,  1]],

         [[-1, -1, -1,  ..., -1, -1,  1],
          [-1,  1,  1,  ...,  1, -1, -1],
          [-1, -1, -1,  ..., -1, -1, -1],
          ...,
          [ 1,  1,  1,  ..., -1, -1,  1],
          [-1, -1, -1,  ..., -1, -1, -1],
          [ 1,  1,  1,  ..., -1, -1,  1]],

         [[-1, -1, -1,  ..., -1, -1,  1],
          [-1,  1,  1,  ...,  1, -1, -1],
          [-1, -1, -1,  ..., -1, -1, -1],
          ...,
          [ 1,  1,  1,  ..., -1, -1,  1],
          [-1, -1, -1,  ..., -1, -1, -1],
          [ 1,  1,  1,  ..., -1, -1,  1]],

         ...,

         [[-1,  1,  1,  ...,  1, -1, -1],
          [ 1,  1,  1,  ...,  1, -1, -1],
          [-1, -1,  1,  ...,  1, -1,  1],
          ...,
          [ 1,  1,  1,  ..., -1,  1,  1],
          [-1,  1,  1,  ...,  1, -1, -1],
          [-1, -1, -1,  ...,  1, -1,  1]],

         [[-1,  1,  1,  ...,  1, -1, -1],
          [ 1,  1,  1,  ...,  1, -1, -1],
          [-1, -1,  1,  ...,  1, -1,  1],
          ...,
          [ 1,  1,  1,  ..., -1,  1,  1],
          [-1,  1,  1,  ...,  1, -1, -1],
          [-1, -1, -1,  ...,  1, -1,  1]],

         [[-1,  1,  1,  ...,  1, -1, -1],
          [ 1,  1,  1,  ...,  1, -1, -1],
          [-1, -1,  1,  ...,  1, -1,  1],
          ...,
          [ 1,  1,  1,  ..., -1,  1,  1],
          [-1,  1,  1,  ...,  1, -1, -1],
          [-1, -1, -1,  ...,  1, -1,  1]]]),
 tensor([ 1.0000e+00,  9.9900e-01,  9.9800e-01,  ...,  2.0000e-03,
          1.0000e-03, -8.8124e-16]))
```

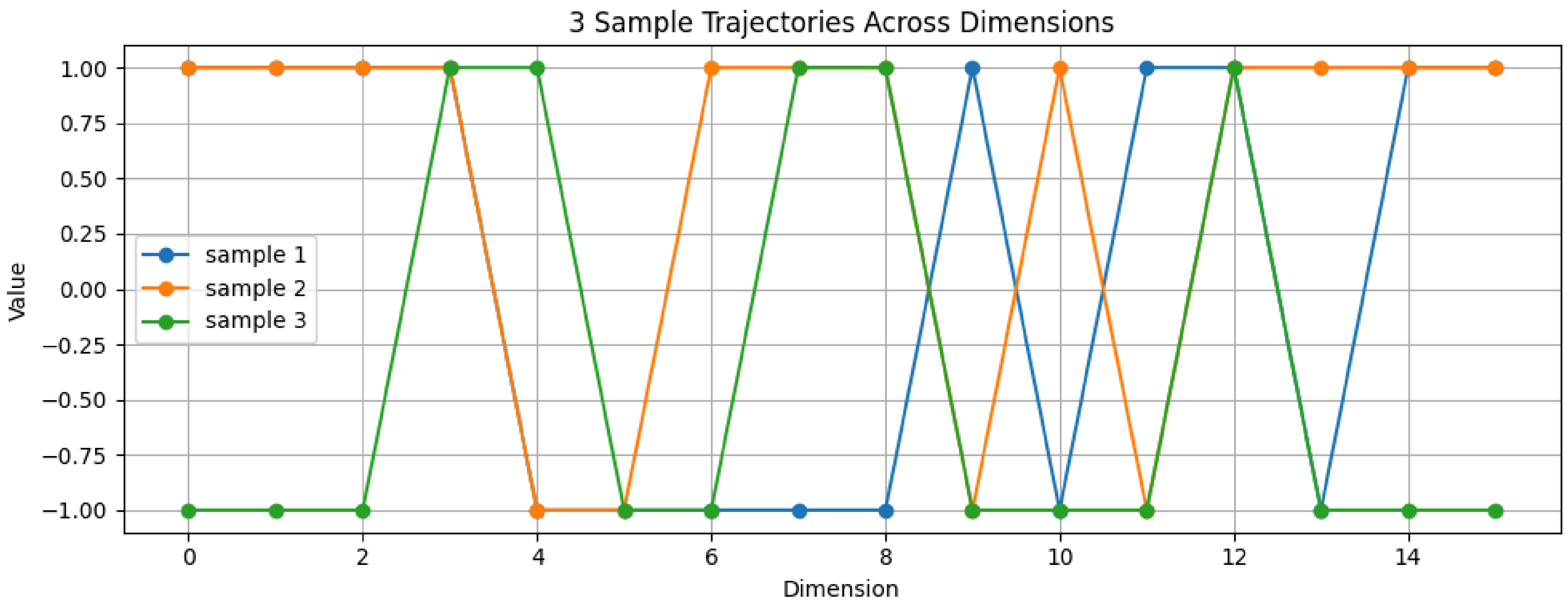
## Training Setup

```
In [13]: # abstract the procedure of setting up a training into a single function
# h is diffusion time step
def setup_train(N, d, h, t1=1, visualize = False):
    samples = sample(N, d)
    if(visualize):
        visualize_sample(samples.detach().numpy())
    layers, ts = forward_sampler(t1, h, samples)
    if(visualize):
        visualize_sample(layers[-1].detach().numpy())
    xs = flatten(layers, ts)
    return xs, samples
```

```
In [14]: def compute_mean_and_cov(arrays):
    """
    Compute the mean and covariance of a list or array of d-dimensional numpy arrays.

    Parameters:
        arrays (np.ndarray): An (n, d) array, where each row is a d-dimensional sample.

    Returns:
        mean (np.ndarray): A (d,) array representing the mean vector.
        cov (np.ndarray): A (d, d) array representing the covariance matrix.
    """
    arrays = np.asarray(arrays)
    # filter out of range
    # arrays = arrays[np.all((arrays > -2.5) & (arrays < 2.5), axis=1)]
    if arrays.ndim != 2:
        raise ValueError("Input should be a 2D array with shape (n_samples, d)")

    mean = np.mean(arrays, axis=0)
    cov = np.cov(arrays, rowvar=False)  # Each row is a sample

    return mean, cov
```

In [15]:
```
xs, x0 = setup_train(10000, 16, 0.001, t1 = 1, visualize=True)
data_mean, data_cov = compute_mean_and_cov(x0.detach().numpy())
print(xs.shape, x0.shape)
del xs
gc.collect()
```





```
torch.Size([10010000, 17]) torch.Size([10000, 16])
```

Out[15]: 4250

## Implementing the network

As we are training a conditional marginal distribution given time $t$,

$$p_t(X^d|x^{\backslash d};\theta),$$

we will minimize functional

$$\theta^* = \text{argmin}_\theta \int_0^T \sum_{x_t\in\chi^n} q_t(x_t)\sum_{d=1}^D \log p_t(X^d = x_t^d|x_t^{\backslash d};\theta)dt.$$

Once we train $p_t(X^d|x^{\backslash d};\theta)$, we obtain approximation to backward rate

$$R_t^d(x,y) = \frac{q_t(y^d,x^{\backslash d})}{q_t(x^d,x^{\backslash d})}Q_t(y,x) \simeq \frac{p_t(y^d|x^{\backslash d};\theta)}{p_t(x^d|x^{\backslash d};\theta)}Q_t(y,x).$$

Note that for each entry $d$, the network should mask the $d$-th dimension input and take the remaining $\chi^{n-1}$ input along with a new category $y\in\chi$, and output a probability.

For the binary state space, we may simplify the interface from $[n]\times\chi^{n-1}\times\chi\times\mathbb{R}\to\mathbb{R}$ to

$$N:\chi^n\times\mathbb{R}\to\mathbb{R}^n,$$

where we implicitly mask the $d$-th input dimension from the conditional marginal for the $d$-th output dimension, and the output probability corresponds to the $+1$ case.

Namely:

$$p_t(X^d = +1|x^{\setminus d}) = N(x,t)[d];$$
$$p_t(X^d = -1|x^{\setminus d}) = 1 - N(x,t)[d].$$

However, due to translational invariance (of the potential), we may simplify the network with the underlying structure of $N$ given by

$$N(x,t)[d] = M(x^{\setminus d}[rotated], t).$$

.

In [16]:
```python
import torch
import torch.nn as nn
import torch.nn.functional as F

# we use a simple linear network to modulate the time dependence
class FiLM(nn.Module):
    def __init__(self, channels, t_dim=1, hidden_dim=16):
        super().__init__()
        self.film = nn.Sequential(
            nn.Linear(t_dim, hidden_dim),
            nn.ReLU(),
            nn.Linear(hidden_dim, channels * 2)  # gamma and beta
        )
        self.channels = channels

    def forward(self, x, t):
        """
        x: [batch, channels, spatial_dim]
        t: [batch, t_dim]
        """
        params = self.film(t)           # [batch, 2*channels]
        gamma, beta = params.chunk(2, dim=-1)  # Each: [batch, channels]
        gamma = gamma.unsqueeze(-1)     # [batch, channels, 1]
        beta = beta.unsqueeze(-1)       # [batch, channels, 1]
        return gamma * x + beta

class RotConvFiLMNetM(nn.Module):
    def __init__(self, n_minus_1, conv_channels=6, kernel_size=3, hidden_dim=32, t_dim=1):
        super().__init__()
        self.n_minus_1 = n_minus_1
        # use convolution on the input
        self.conv = nn.Conv1d(
            in_channels=1,
            out_channels=conv_channels,
            kernel_size=kernel_size,
            padding=kernel_size // 2,
            padding_mode='circular'
        )
        self.conv2 = nn.Conv1d(
            in_channels=conv_channels,
            out_channels=1,
            kernel_size=kernel_size,
            padding=kernel_size // 2,
            padding_mode='circular'
        )

        self.film = FiLM(conv_channels, t_dim, hidden_dim)
        self.fc = nn.Sequential(
            nn.Linear(n_minus_1, hidden_dim),
            nn.ReLU(),
            nn.Linear(hidden_dim, 1),
            nn.Sigmoid()
        )

    def forward(self, x_spatial, t):
        """
        x_spatial: [batch, n-1], entries in {-1, 1}
        t: [batch, 1], float
        """
        x = x_spatial.unsqueeze(1)        # [batch, 1, n-1]

        conv_out = self.conv(x)           # [batch, conv_channels, n-1]
        conv_out = self.film(conv_out, t) # Modulate by time!
        conv_out = F.silu(conv_out)       # add in non-linearity
        conv_out = self.conv2(conv_out)[:,0,:]    # [batch, conv_chanels, n-1] -> [batch, n-1]
        out = self.fc(conv_out)             # [batch, 1], in (0,1)
        return out.squeeze(-1)            # [batch]
```

```
class MaskedWrapperN(nn.Module):
    """
    Wraps a module M(x_masked, t) -> scalar
    to apply it to all sites in x.
    """
    def __init__(self, d):
        super().__init__()
        self.M =  RotConvFiLMNetM(d-1) # Any nn.Module: takes (x_masked, t) and returns [batch] or [batch,1]


    def forward(self, xt):
        x = xt[:, :-1]
        t = xt[:, -1].unsqueeze(1)
        """
        x: [batch, n], entries in {-1,1}
        t: [batch, 1]
        Output: [batch, n], N(x, t)[d] = M(x^{\backslash d}, t)
        """
        batch, n = x.shape
        outputs = []
        for d in range(n):
            # Roll so that the entry d%n is now at index 0
            x_rolled = torch.roll(x, shifts= -(d%n), dims=1)  # [batch, n]
            # print(x_rolled[:,0]-x[:,d])
            # Remove the first entry, so we get [x_{d+2}, ..., x_{d}, ...]
            x_masked = x_rolled[:, 1:]   # [batch, n-1]
            x_masked = x_masked / n      # (optional normalization)
            y_d = self.M(x_masked, t)    # [batch]
            outputs.append(y_d.unsqueeze(1))
        out = torch.cat(outputs, dim=1)
        return out
```

The loss simplifies into for sample space $S \subset \chi^n \times T$

$$\begin{aligned}
\theta^* &= \text{argmin}_\theta \int_0^T \sum_{x_t \in \chi^n} q_t(x_t) \sum_{d=1}^{D} -\log p_t(X^d = x_t^d | x_t^{\backslash d}; \theta) dt \\
&= \text{argmin}_\theta \sum_{x_t \in S} \sum_{d=1}^{D} -\log p_t(X^d = x_t^d | x_t^{\backslash d}; \theta) \\
&= \text{argmin}_\theta \sum_{x_t \in S} \sum_{d=1}^{D} -\log\left(\frac{1}{2} - \frac{1}{2} x_t^d + x_t^d N(x,t)[d]\right) \\
&= \text{argmin}_\theta \sum_{x_t \in S} \text{sum}\left(-\log\left(\frac{1}{2} - \frac{1}{2} x_t + x_t * N(x,t)\right), \text{axis} = -1\right)
\end{aligned}$$

In [17]:
```
# compute loss on scores
def compute_loss(xs, model):
    n = xs.shape[0]
    d = xs.shape[1] - 1
    ns = model(xs)
    # print(0.5+xs[:,:-1]*(ns-0.5))
    # print("train: ", xs[5,:-1])
    # print("out: ", ns[5,:-1])
    # print("error: ", 0.5+xs[:,:-1]*(ns-0.5))
    # normalize error by dimension for consistency
    return -torch.log(0.5+xs[:,:-1]*(ns-0.5)).sum()/d/n

def train(N, d, h, t1 = 1, B = 100, model=None, epsilon=1e-4, max_steps=10000):
    xs, x0 = setup_train(N, d, h, t1 = t1)
    if(model == None):
        model = MaskedWrapperN(d)
    optimizer = torch.optim.Adam(model.parameters(), lr=1e-3)

    for step in range(max_steps):
        idx = torch.randint(0, xs.shape[0], (B,))
        batch = xs[idx]
        loss = compute_loss(batch, model)
        optimizer.zero_grad()
        loss.backward()

        if(step%(min(max_steps//10, 100))==0):
            # Compute total gradient norm
            grad_norm = 0.0
            for p in model.parameters():
                if p.grad is not None:
                    grad_norm += p.grad.norm().item()**2
            grad_norm = grad_norm**0.5

            # Check termination condition
            if grad_norm < epsilon or loss<-4:
                print(f"Stopping early at step {step}, grad norm {grad_norm:.2e}")
                break

            print(f'training {step} step with loss {loss}')
        optimizer.step()

    return model, xs
```

In [ ]:
```
masked_p, xs = train(1000, 16, 0.005, t1 = 1, B  = 100, max_steps = 5000)
```

```
training 0 step with loss 0.6993951201438904
training 100 step with loss 0.6930335760116577
training 200 step with loss 0.6886628866195679
training 300 step with loss 0.6554592847824097
training 400 step with loss 0.6353268623352051
training 500 step with loss 0.6430647969245911
training 600 step with loss 0.6202414035797119
training 700 step with loss 0.6317144632339478
training 800 step with loss 0.6125868558883667
training 900 step with loss 0.6374459266662598
training 1000 step with loss 0.6229844689369202
training 1100 step with loss 0.6295598745346069
training 1200 step with loss 0.613991379737854
training 1300 step with loss 0.6158667206764221
training 1400 step with loss 0.6371795535087585
training 1500 step with loss 0.6429629325866699
training 1600 step with loss 0.6274345517158508
training 1700 step with loss 0.6409488916397095
training 1800 step with loss 0.6264355182647705
training 1900 step with loss 0.6353839039802551
training 2000 step with loss 0.6245768070220947
training 2100 step with loss 0.6293175220489502
training 2200 step with loss 0.6164796352386475
training 2300 step with loss 0.6093201637268066
training 2400 step with loss 0.6242440938949585
training 2500 step with loss 0.6129231452941895
training 2600 step with loss 0.6255311369895935
training 2700 step with loss 0.6314204931259155
training 2800 step with loss 0.6342000365257263
training 2900 step with loss 0.635718822479248
training 3000 step with loss 0.6388227343559265
training 3100 step with loss 0.6247830986976624
training 3200 step with loss 0.6161007881164551
training 3300 step with loss 0.6281055808067322
training 3400 step with loss 0.6176475882530212
training 3500 step with loss 0.6355020999908447
training 3600 step with loss 0.5880162715911865
training 3700 step with loss 0.6264427304267883
training 3800 step with loss 0.6326869130134583
training 3900 step with loss 0.6154675483703613
training 4000 step with loss 0.6376744508743286
training 4100 step with loss 0.6251152157783508
training 4200 step with loss 0.6402712464332581
training 4300 step with loss 0.6371673345565796
training 4400 step with loss 0.6174423694610596
training 4500 step with loss 0.6213792562484741
training 4600 step with loss 0.6244871020317078
training 4700 step with loss 0.6228694319725037
training 4800 step with loss 0.6393604278564453
training 4900 step with loss 0.6648422479629517
```

In [ ]:
```
masked_p(xs[[0,90,1000,5020,30],:])
```

Out[ ]:
```
tensor([[0.3820, 0.3820, 0.4694, 0.4694, 0.3891, 0.4761, 0.3895, 0.4761, 0.3895,
          0.4761, 0.3895, 0.4761, 0.3891, 0.4698, 0.4698, 0.4698],
         [0.3996, 0.3174, 0.3957, 0.3141, 0.3141, 0.3141, 0.3924, 0.3924, 0.3924,
          0.3167, 0.3924, 0.3924, 0.3924, 0.3924, 0.3924, 0.3171],
         [0.8387, 0.8387, 0.8802, 0.8802, 0.8387, 0.8387, 0.8387, 0.8387, 0.8387,
          0.8387, 0.8387, 0.8387, 0.8387, 0.8387, 0.8387, 0.8387],
         [0.5981, 0.5981, 0.6534, 0.6534, 0.6534, 0.6534, 0.6001, 0.6553, 0.5981,
          0.5981, 0.5981, 0.6526, 0.5981, 0.5981, 0.5981, 0.5981],
         [0.3174, 0.4000, 0.4000, 0.4000, 0.4000, 0.4000, 0.3236, 0.3996, 0.3996,
          0.3210, 0.3210, 0.3210, 0.4000, 0.4000, 0.4000, 0.3174]],
        grad_fn=<CatBackward0>)
```

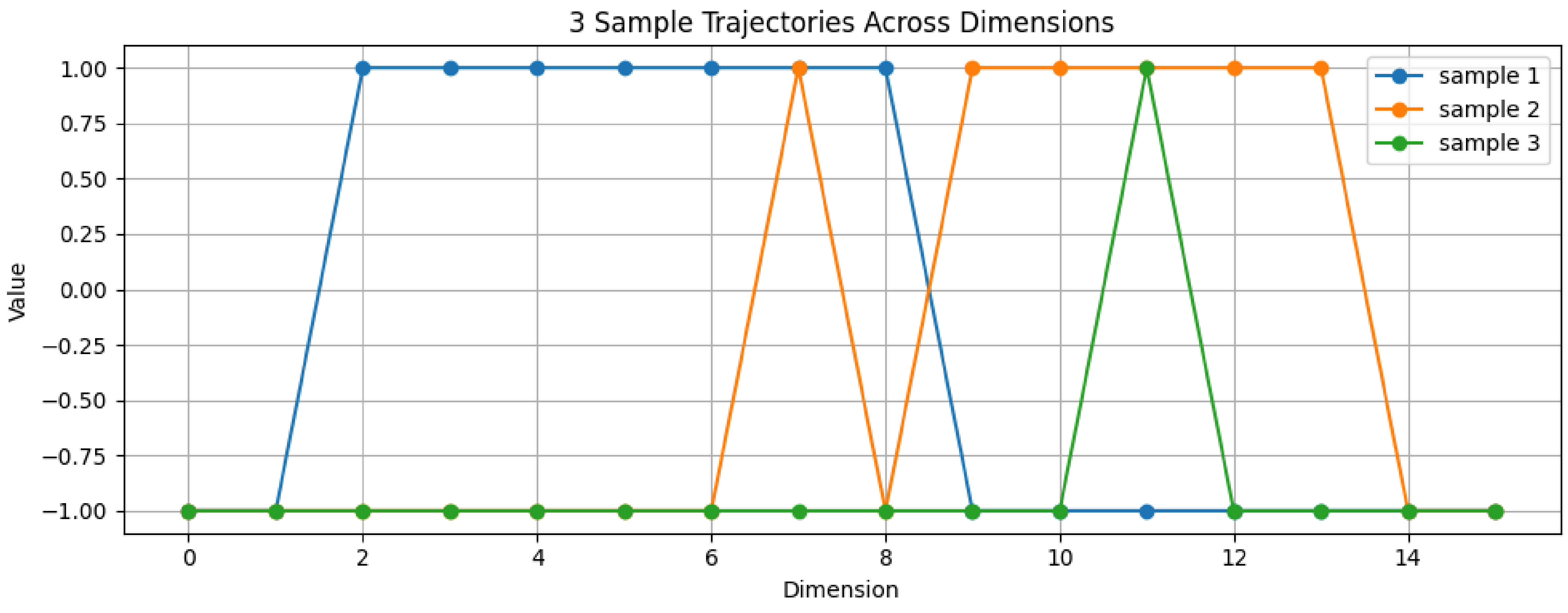
During inverse diffusion, we make the following computations:

$$p^d_{t+\epsilon|t}(X^d_{t+\epsilon} = c \,|\, x^{\backslash d}_t; \theta) = \begin{cases} \epsilon\, R^d_t\left(x_t,\, x^d_{t+\epsilon} = c;\, \theta\right) & \text{if } c \neq x^d_t \\ 1 - \epsilon\, R^d_t\left(x_t,\, x^d_{t+\epsilon} = -c;\, \theta\right) & \text{otherwise} \end{cases}$$

In [ ]:
```
# Eulerian Backward Diffusion Sampler (Fully Vectorized, Batches All Dimensions)
import torch

def stable_diffusion(masked_prbs, d, N, h, t1, device=None):
    """
    masked_prbs: function mapping (N x (d+1)) input to (N x d) probabilities
    d: dimension
    N: batch size
    h: time step
    t1: total time
    device: torch device
    mean: mean for output shift (default 0)
    """
    if device is None:
        device = torch.device('cpu')

    t = 0.0
    y0 = torch.randint(0, 2, (N, d), device=device, dtype=torch.float32)
    y = (y0 * 2 - 1)

    Q, P, eigvals = diagonalize_Q(2)
    Q_off_diag = float(Q[0, 1])  # flip rate

    while t <= t1 + 1e-6:
        x = torch.cat((y, torch.full((N, 1), t, dtype=y.dtype, device=device)), dim=1)
        ns = masked_prbs(x)  # (N x d), probability of +1 for each bit

        p_plus = ns
        p_minus = 1 - ns
        curr_val = y

        # For each entry, p_flip = p_plus if y == -1 else p_minus
        p_flip = torch.where(curr_val == 1, p_minus, p_plus)
        p_stay = torch.where(curr_val == 1, p_plus, p_minus)

        R = Q_off_diag * p_flip / (p_stay + 1e-12)
        flip_prob = h * R
        flip_prob = torch.clamp(flip_prob, 0, 1)

        flip = torch.rand(N, d, device=device) < flip_prob
        y[flip] *= -1

        t += h
    return y
```

In [ ]:
```
ys = stable_diffusion(masked_p, 16, 10000, 0.01, 1)
ys = ys.detach().numpy()
```

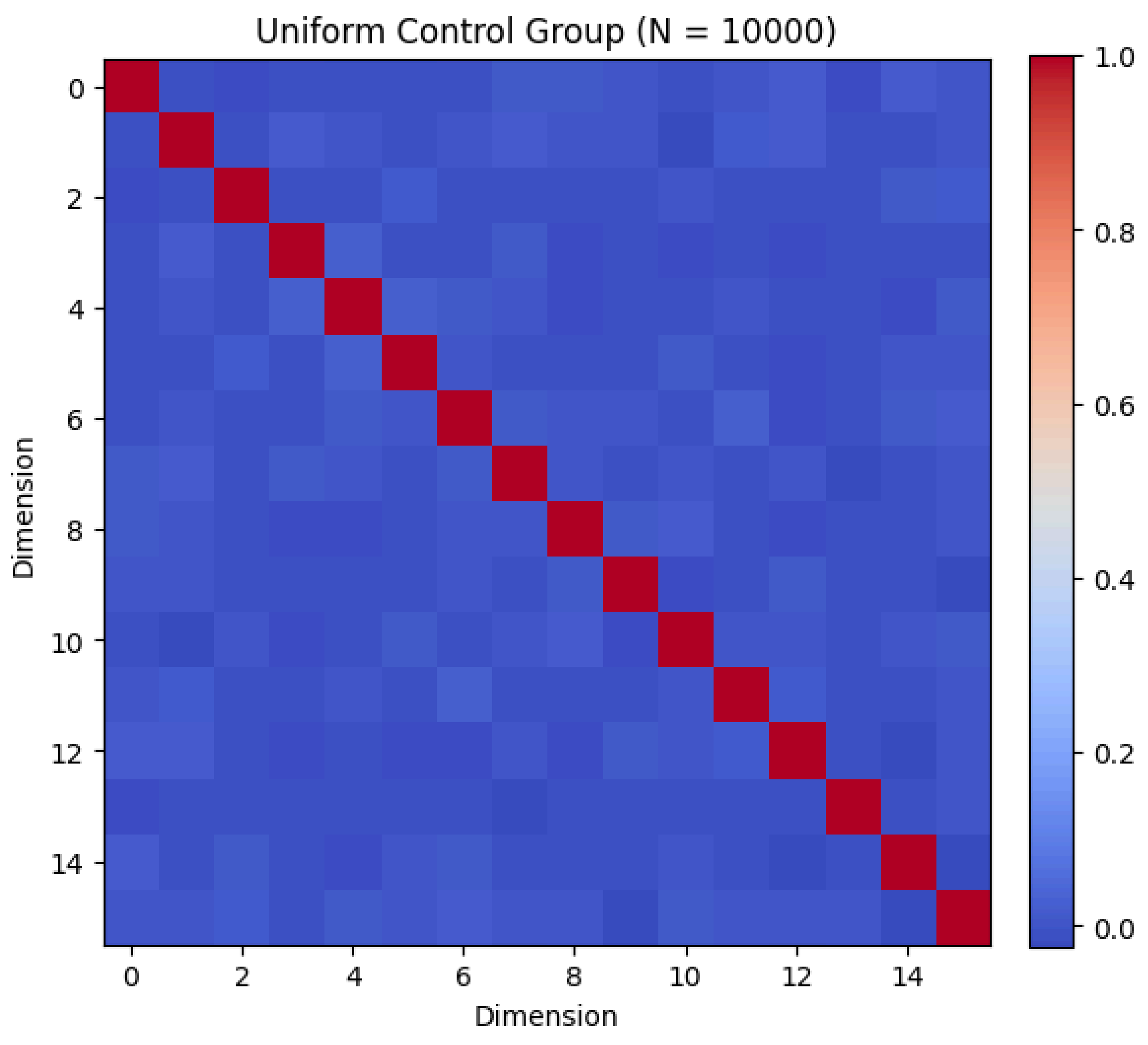
In [ ]:
```
visualize_sample(ys,3)
```

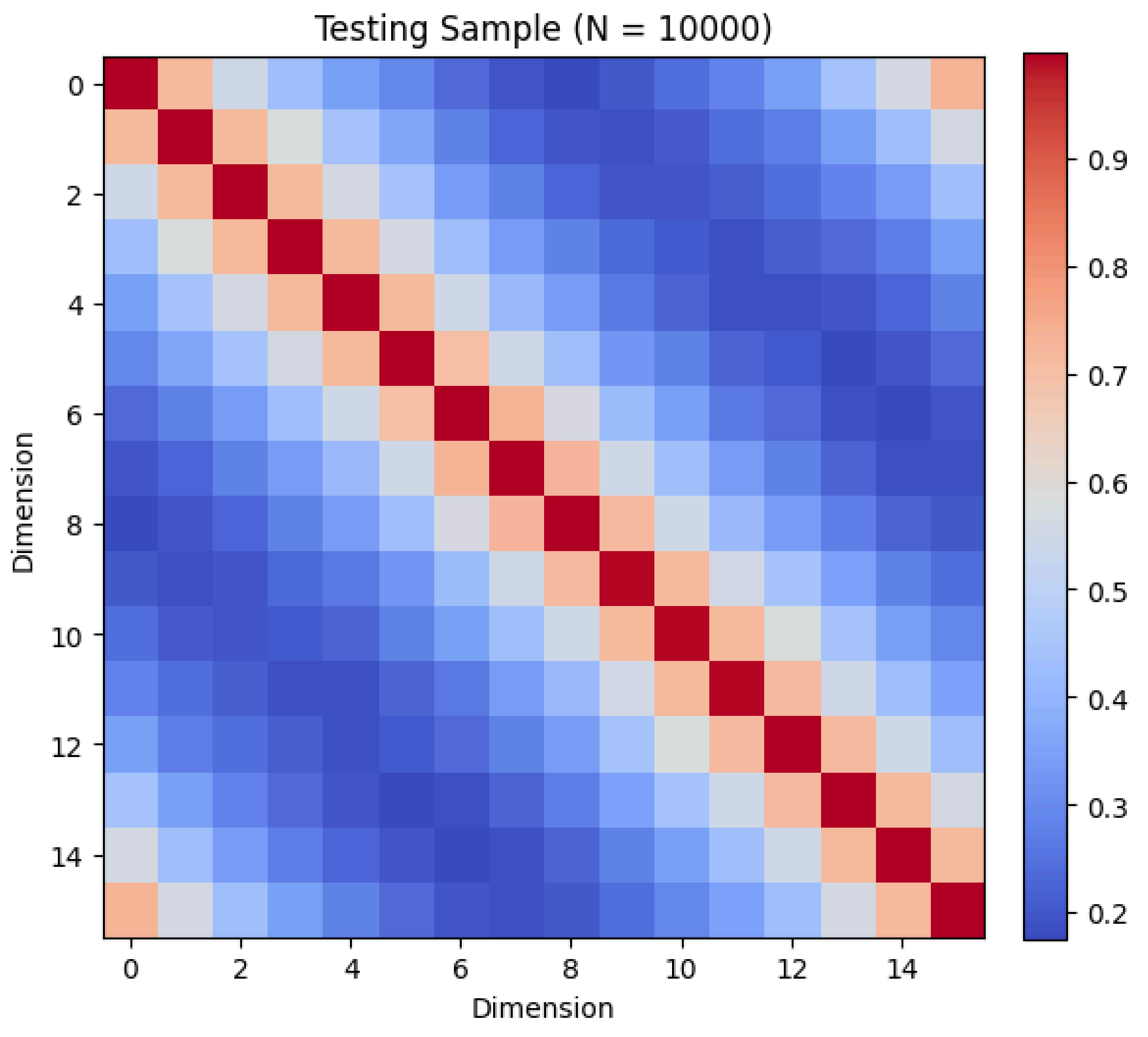


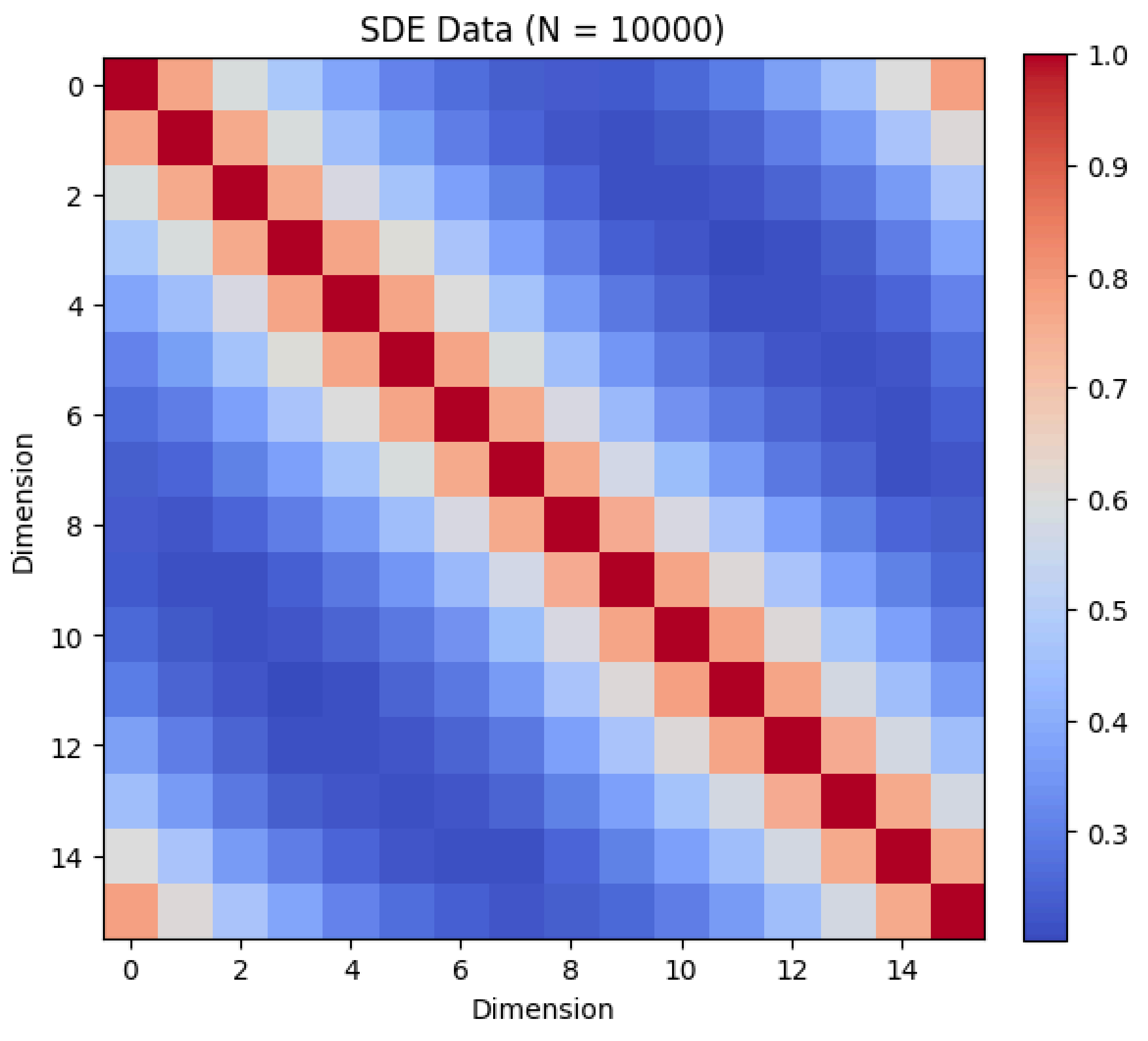
It seems for some of the samples, the distribution looks quite convincing.

We will proceed to comparing the covariance and mean:

In [ ]:
```
import matplotlib.pyplot as plt
import numpy as np

def plot_cov_matrix(cov, ax=None, labels=None, title="Covariance Matrix"):
    """
    Plot a covariance matrix as a heatmap.

    Parameters:
        cov (np.ndarray): (d, d) covariance matrix.
        ax (matplotlib.axes.Axes, optional): Axis to plot on.
        labels (list, optional): List of d labels for axis ticks.
        title (str): Title of the plot.
    """
    if ax is None:
        fig, ax = plt.subplots(figsize=(6,6))
    im = ax.imshow(cov, cmap='coolwarm', interpolation='nearest')
    plt.colorbar(im, ax=ax, fraction=0.046, pad=0.04)
    d = cov.shape[0]
    if labels is not None:
        ax.set_xticks(np.arange(d))
        ax.set_yticks(np.arange(d))
        ax.set_xticklabels(labels)
        ax.set_yticklabels(labels)
    ax.set_title(title)
    ax.set_xlabel("Dimension")
    ax.set_ylabel("Dimension")
    plt.tight_layout()
    plt.show()

mean_uniform, cov_uniform = compute_mean_and_cov(2 * np.random.randint(0, 2, size=(10000,16)) - 1)
plot_cov_matrix(cov_uniform, title='Uniform Control Group (N = 10000)')

mean_trained, cov_trained = compute_mean_and_cov(ys)
plot_cov_matrix(cov_trained, title='Testing Sample (N = 10000)')

mean_data, cov_data = compute_mean_and_cov(x0)
plot_cov_matrix(cov_data, title='SDE Data (N = 10000)')
```







In [ ]:
```python
print(f"Trained mean: {mean_trained}")
# print(f"Trained covariance: {cov_trained}")
print(f"Data mean: {mean_data}")
# print(f"Data covariance: {cov_data}")
print(f"Mean Error: {np.linalg.norm(mean_trained)}")
print(f"Covariance Error: {np.linalg.norm(cov_trained - cov_data)}")
print(f"Uniform Covariance Error: {np.linalg.norm(cov_uniform - cov_data)}")
```

```
Trained mean: [0.0654 0.0668 0.059  0.0488 0.061  0.0728 0.0742 0.068  0.0746 0.0792
 0.0774 0.075  0.0736 0.0688 0.0548 0.0704]
Data mean: [ 0.0052  0.0108  0.004   0.001   0.004   0.0006  0.005   0.0056  0.0082
  0.0218  0.0208  0.0154  0.0204  0.0122  0.0042 -0.0028]
Mean Error: 0.2744366526603699
Covariance Error: 0.487388104978924
Uniform Covariance Error: 6.935428244571773
```

As we may observe, the network with two convolution layers modulated by a FiLM layer in between, then passed into a fully connected layer was capable of learning the distribution on a sample size of 1000 with diffusion step size 0.05. **The convariance error between the training and testing data was 0.487, compared to the covariance error between a uniformly generated random sample and the training data which is as high as 6.954. The mean error was also close to 0.** We expect to see a further decrease in error with training sample size increased to near 10000.

We shall continue to constructing the experiment for $(N, d) \in \{20^2, 40^2, 60^2, 80^2, 100^2\} \times \{16, 32, 64, 128\}$ for a more thorough comparison.

## (a)

Compare the sample mean and covariance obtained from the score based di usion model with those from the SDE simulation. Use di erent values of N. Do you see the error decay as $\frac{1}{\sqrt{N}}$?

In [19]:
```python
# GPU Ready:
def train_gpu(N, d, h, t1 = 1, B = 100, model=None, epsilon=1e-4, max_steps=10000):
    device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
    print(f"Using device: {device}")

    xs, x0 = setup_train(N, d, h, t1 = t1)
    xs = xs.to(device)
    x0 = x0.to(device) # Move x0 to GPU if needed later

    if model is None:
        model = MaskedWrapperN(d).to(device)
    else:
        model = model.to(device) # Move existing model to GPU

    optimizer = torch.optim.Adam(model.parameters(), lr=1e-3)

    for step in range(max_steps):
        idx = torch.randint(0, xs.shape[0], (B,), device=device)
        batch = xs[idx]
        loss = compute_loss(batch, model)

        optimizer.zero_grad()
        loss.backward()

        if(step%(min(max_steps//10, 100))==0):
            # Compute total gradient norm
            grad_norm = 0.0
            for p in model.parameters():
                if p.grad is not None:
                    grad_norm += p.grad.norm().item()**2
            grad_norm = grad_norm**0.5

            # Check termination condition
            # Move loss to CPU for printing/comparison if on GPU
            current_loss = loss.item()
            if grad_norm < epsilon or current_loss < -4:
                print(f"Stopping early at step {step}, grad norm {grad_norm:.2e}")
                break

            print(f'training {step} step with loss {current_loss}')
        optimizer.step()

    # Move model back to CPU if desired after training, or keep on GPU for inference
    # model = model.to('cpu')
    # xs = xs.to('cpu')
    # x0 = x0.to('cpu')

    return model, xs
```

In [18]:
```python
# GPU Ready:

def stable_diffusion_gpu(masked_prbs, d, N, h, t1, device=None):
    """
    Eulerian Backward Diffusion Sampler (Fully Vectorized, Batches All Dimensions)
    GPU Ready version.

    masked_prbs: function mapping (N x (d+1)) input to (N x d) probabilities.
                 Should be a torch.nn.Module that runs on the specified device.
    d: dimension
    N: batch size
    h: time step
    t1: total time
    device: torch device (e.g., 'cuda', 'cpu')
    """
    if device is None:
        device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')

    # Move the model to the specified device
    # Assuming masked_prbs is a torch.nn.Module
    masked_prbs.to(device)

    t = 0.0
    # Initialize on the specified device
    y0 = torch.randint(0, 2, (N, d), device=device, dtype=torch.float32)
    y = (y0 * 2 - 1)

    # diagonalize_Q returns numpy arrays, convert to torch tensors on device
    Q_np, P_np, eigvals_np = diagonalize_Q(2)
    Q = torch.tensor(Q_np, dtype=torch.float64, device=device)
    # P and eigvals are not directly used in the loop, only Q_off_diag
    Q_off_diag = float(Q[0, 1])  # flip rate

    # Convert Q_off_diag back to tensor if needed in calculations, but float is fine here

    while t <= t1 + 1e-6:
        # Ensure all tensors used in the forward pass are on the same device
        x = torch.cat((y, torch.full((N, 1), t, dtype=y.dtype, device=device)), dim=1)

        # Call the masked_prbs model
        with torch.no_grad(): # Inference mode for sampling
            ns = masked_prbs(x)  # (N x d), probability of +1 for each bit

        p_plus = ns
        p_minus = 1 - ns
        curr_val = y

        # For each entry, p_flip = p_plus if y == -1 else p_minus
        p_flip = torch.where(curr_val == 1, p_minus, p_plus)
        p_stay = torch.where(curr_val == 1, p_plus, p_minus)

        # Ensure Q_off_diag is a tensor on device for calculation
        R = torch.tensor(Q_off_diag, device=device) * p_flip / (p_stay + 1e-12)
        flip_prob = h * R
        flip_prob = torch.clamp(flip_prob, 0, 1)

        # Generate random numbers on the same device
        flip = torch.rand(N, d, device=device) < flip_prob
        y[flip] *= -1

        t += h

    return y
```

In [23]:
```
# prompt: please simplify the run experiment for d logic by reusing previously defined train_gpu

import gc # Import the garbage collection module

def run_experiment_for_d(d, N_values, h = 0.005, inf_h = 0.005, t1=1, use_trained = False, max_steps_per_logN=1000):
    """
    Runs experiment (a) comparing sample mean and covariance for different N values.

    Args:
        N_values (list): List of N values to test.
        d (int): Dimension of the samples.
        h (float): Diffusion step size.
        t1 (float): Final diffusion time.
        max_steps_per_N (int): Maximum training steps for each N value.
    """
    mean_errors = []
    cov_errors = []

    # Generate initial data for comparison outside the loop for efficiency
    # Assuming the target distribution doesn't change with N, only sample size does
    # We need a large reference set to compare against
    x0 = sample(100000, d)
    data_mean_ref, data_cov_ref = compute_mean_and_cov(x0.detach().numpy())
    del x0
    print("Reference data generated.")

    for N in N_values:
        print(f"\n--- Running experiment for N = {N}, d = {d} ---")

        # Reuse the train_gpu function
        # We will re-initialize the model and optimizer for each N unless specified otherwise
        masked_p = MaskedWrapperN(d)
        optimizer = None # Let train_gpu create a new optimizer
        # Adjust max_steps based on N if needed, or keep constant
        current_max_steps = int(max_steps_per_logN*np.log10(N)) # Could scale with log(N) or sqrt(N)
        model = masked_p
        if(use_trained):
          masked_p.load_state_dict(torch.load(f'masked_p{d}_{N}.pth'))
          # run this step to restore initial mean and variance estimations
        else:
          # train for two epochs
          # first pretrain on small batches
            # train(1000, 16, 0.005, t1 = 1, B  = 100, max_steps = 5000)
          model, xs = train_gpu(
              N, d, h, t1=t1,
              model=masked_p,
              B= N//10,
              max_steps=current_max_steps
          )

        del xs
        torch.cuda.empty_cache()
        gc.collect()

        torch.save(masked_p.state_dict(), f'masked_p{d}_{N}.pth')

        print(f"Training finished for N = {N}.")

        # Generate samples from the trained model
        N_generate = 10000 # Generate a fixed large number of samples for consistent evaluation
        print(f"Generating {N_generate} samples from the trained model for N = {N}.")
        ys_batches = []
        batch_size_inf = 1000 # Smaller batch size for inference if memory is an issue

        # batch compute samples
        for i in range(N_generate // batch_size_inf):

          ys = stable_diffusion_gpu(
              model,
              d=d,
              N=batch_size_inf,
              h=inf_h, # Inference step size can be different from training h
              t1=t1
          )
          ys_cpu = ys.cpu().detach().numpy()
          ys_batches.append(ys_cpu)

          del ys

          # make sure that there is enough memory in GPU
          torch.cuda.empty_cache()
          gc.collect()

        print(f"Sample generation finished for N = {N}.")
        ys_all = np.concatenate(ys_batches, axis=0)
        print(f"Concatenation finished for N = {N}.")

        # Compute mean and covariance of the generated samples
        trained_mean, trained_cov = compute_mean_and_cov(ys_all)

        del ys_all
        torch.cuda.empty_cache()
        gc.collect()

        # Compute errors relative to the reference data
        mean_error = np.linalg.norm(trained_mean - data_mean_ref)
        cov_error = np.linalg.norm(trained_cov - data_cov_ref) # Frobenius norm

        mean_errors.append(mean_error)
        cov_errors.append(cov_error)

        print(f"N = {N}: Mean Error = {mean_error:.4e}, Covariance Error = {cov_error:.4e}")

    return mean_errors, cov_errors, N_values
```

In [24]:
```
def plot_errors(N_values, mean_errors, cov_errors, d_val):
    """Plots mean and covariance errors against N on regular and log-log scales."""
    N_values_np = np.array(N_values)
    mean_errors_np = np.array(mean_errors)
    cov_errors_np = np.array(cov_errors)

    fig, axes = plt.subplots(1, 2, figsize=(14, 6))

    # Regular plot
    axes[0].plot(N_values_np, mean_errors_np, marker='o', label='Mean Error')
    axes[0].plot(N_values_np, cov_errors_np, marker='x', label='Covariance Error')
    axes[0].set_xlabel('Sample Size (N)')
    axes[0].set_ylabel('Error (Frobenius Norm)')
    axes[0].set_title(f'Error vs. Sample Size (d={d_val}) - Regular Scale')
    axes[0].legend()
    axes[0].grid(True)

    # Log-log plot
    axes[1].loglog(N_values_np, mean_errors_np, marker='o', label='Mean Error')
    axes[1].loglog(N_values_np, cov_errors_np, marker='x', label='Covariance Error')
    # Add theoretical O(1/sqrt(N)) decay line
    # Choose a reference point and plot decay relative to it
    if len(N_values) > 1:
      N_ref = N_values_np[1]
      mean_err_ref = mean_errors_np[1]
```

```
        cov_err_ref = cov_errors_np[1]
        axes[1].loglog(N_values_np, mean_err_ref * np.sqrt(N_ref / N_values_np), linestyle='--', color='gray', label=r'$O(1/\sqrt{N})$
        axes[1].loglog(N_values_np, cov_err_ref * np.sqrt(N_ref / N_values_np), linestyle=':', color='purple', label=r'$O(1/\sqrt{N})$

    axes[1].set_xlabel('Sample Size (N)')
    axes[1].set_ylabel('Error (Frobenius Norm)')
    axes[1].set_title(f'Error vs. Sample Size (d={d_val}) - Log-Log Scale')
    axes[1].legend()
    axes[1].grid(True, which="both", ls="-")

    plt.tight_layout()
    plt.show()
```

In [25]:
```
# Define experiment parameters
N_values = [400, 1600, 3600, 6400, 10000]
# d_values = [16, 32, 64, 128]

# Run experiments for each d
# test first
mean_errors_16, cov_errors_16, N_experiment_16 = run_experiment_for_d(16, N_values,max_steps_per_logN=1500)
%store mean_errors_16
%store cov_errors_16
%store N_experiment_16

mean_errors_32, cov_errors_32, N_experiment_32 = run_experiment_for_d(32, N_values,max_steps_per_logN=1500)
%store mean_errors_32
%store cov_errors_32
%store N_experiment_32

mean_errors_64, cov_errors_64, N_experiment_64 = run_experiment_for_d(64, N_values,max_steps_per_logN=1500)
%store mean_errors_64
%store cov_errors_64
%store N_experiment_64

mean_errors_128, cov_errors_128, N_experiment_128 = run_experiment_for_d(128, N_values,max_steps_per_logN=1500)
%store mean_errors_128
%store cov_errors_128
%store N_experiment_128
```

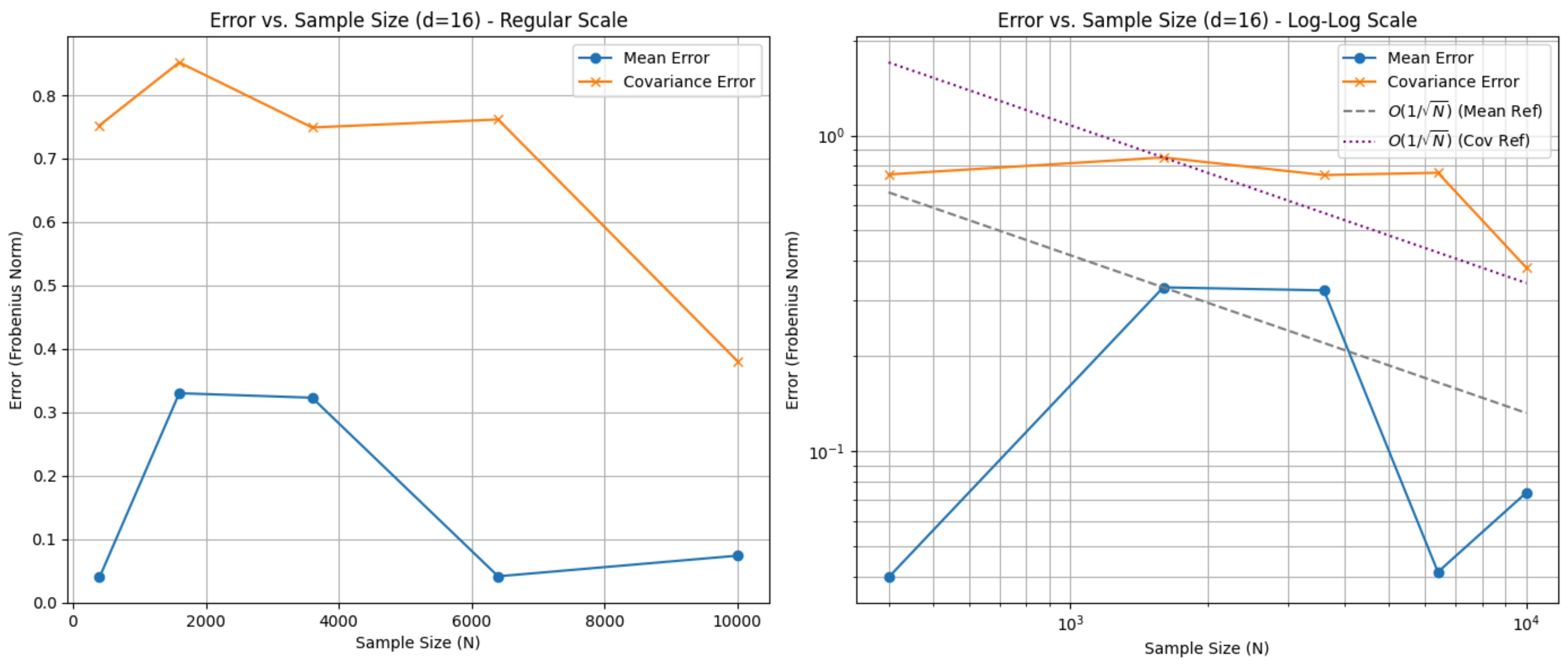
```
Reference data generated.

--- Running experiment for N = 400, d = 16 ---
Using device: cuda
training 0 step with loss 0.6963979601860046
training 100 step with loss 0.6926891803741455
training 200 step with loss 0.6911597847938538
training 300 step with loss 0.5990937352180481
training 400 step with loss 0.6205127239227295
training 500 step with loss 0.5903016924858093
training 600 step with loss 0.6574484705924988
training 700 step with loss 0.6120573282241821
training 800 step with loss 0.6042596697807312
training 900 step with loss 0.6441349983215332
training 1000 step with loss 0.6380757093429565
training 1100 step with loss 0.609254002571106
training 1200 step with loss 0.6159709095954895
training 1300 step with loss 0.6568394899368286
training 1400 step with loss 0.6317651867866516
training 1500 step with loss 0.6132981181144714
training 1600 step with loss 0.6110690236091614
training 1700 step with loss 0.5762380957603455
training 1800 step with loss 0.5993508696556091
training 1900 step with loss 0.6567398905754089
training 2000 step with loss 0.6351074576377869
training 2100 step with loss 0.6621373891830444
training 2200 step with loss 0.6426971554756165
training 2300 step with loss 0.6463287472724915
training 2400 step with loss 0.5868980288505554
training 2500 step with loss 0.6645302176475525
training 2600 step with loss 0.6162987947463989
training 2700 step with loss 0.5967734456062317
training 2800 step with loss 0.6202970147132874
training 2900 step with loss 0.5693133473396301
training 3000 step with loss 0.6272256970405579
training 3100 step with loss 0.6350017786026001
training 3200 step with loss 0.6094204783439636
training 3300 step with loss 0.6200193762779236
training 3400 step with loss 0.5614008903503418
training 3500 step with loss 0.6417177319526672
training 3600 step with loss 0.5796269178390503
training 3700 step with loss 0.6520849466323853
training 3800 step with loss 0.6751441955566406
training 3900 step with loss 0.592857837677002
Training finished for N = 400.
Generating 10000 samples from the trained model for N = 400.
```

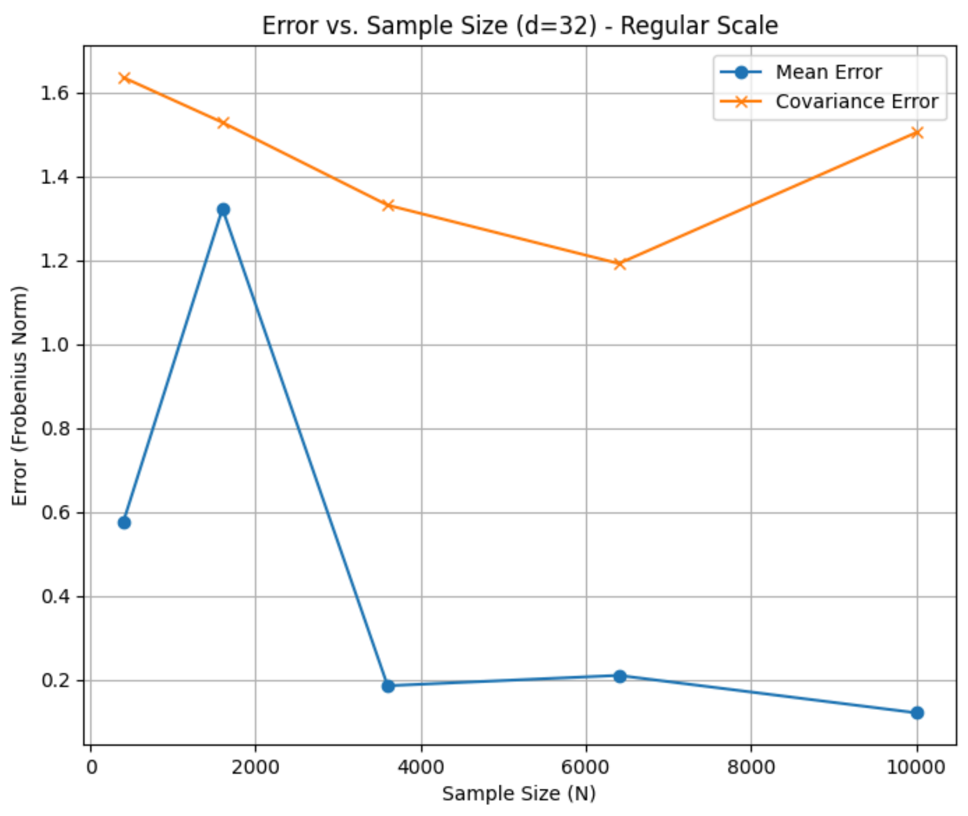
```
training 5900 step with loss 0.6237167716026306
Training finished for N = 10000.
Generating 10000 samples from the trained model for N = 10000.
Sample generation finished for N = 10000.
Concatenation finished for N = 10000.
N = 10000: Mean Error = 3.9146e-01, Covariance Error = 1.4585e+00
Stored 'mean_errors_64' (list)
Stored 'cov_errors_64' (list)
Stored 'N_experiment_64' (list)
Reference data generated.

--- Running experiment for N = 400, d = 128 ---
Using device: cuda
training 0 step with loss 0.693362295627594
training 100 step with loss 0.6929059028625488
training 200 step with loss 0.6932384371757507
training 300 step with loss 0.6932101845741272
training 400 step with loss 0.6931857466697693
training 500 step with loss 0.6931503415107727
training 600 step with loss 0.6932057738304138
training 700 step with loss 0.6931678652763367
training 800 step with loss 0.6930814385414124
training 900 step with loss 0.6932483911514282
training 1000 step with loss 0.693285346031189
training 1100 step with loss 0.6931585669517517
training 1200 step with loss 0.6931187510490417
training 1300 step with loss 0.6787585616111755
training 1400 step with loss 0.6237311363220215
training 1500 step with loss 0.6397201418876648
training 1600 step with loss 0.6430363059043884
training 1700 step with loss 0.6004851460456848
training 1800 step with loss 0.6213290095329285
training 1900 step with loss 0.6298896074295044
training 2000 step with loss 0.6060472130775452
training 2100 step with loss 0.6519760489463806
training 2200 step with loss 0.6265531778335571
training 2300 step with loss 0.6178910136222839
training 2400 step with loss 0.6156882643699646
training 2500 step with loss 0.6345596313476562
training 2600 step with loss 0.6458861231803894
training 2700 step with loss 0.602871835231781
training 2800 step with loss 0.5965815782546997
training 2900 step with loss 0.6301807165145874
training 3000 step with loss 0.6467849612236023
training 3100 step with loss 0.6047672629356384
training 3200 step with loss 0.6229720115661621
training 3300 step with loss 0.6389533877372742
training 3400 step with loss 0.589827835559845
training 3500 step with loss 0.6081302762031555
training 3600 step with loss 0.6189838647842407
training 3700 step with loss 0.593726396560669
training 3800 step with loss 0.6360303163528442
training 3900 step with loss 0.6045159697532654
Training finished for N = 400.
Generating 10000 samples from the trained model for N = 400.
Sample generation finished for N = 400.
Concatenation finished for N = 400.
N = 400: Mean Error = 6.3266e-01, Covariance Error = 3.2229e+00

--- Running experiment for N = 1600, d = 128 ---
Using device: cuda
training 0 step with loss 0.6948370933532715
training 100 step with loss 0.6931065917015076
training 200 step with loss 0.6931528449058533
training 300 step with loss 0.6932188868522644
training 400 step with loss 0.693123996257782
training 500 step with loss 0.6527414321899414
training 600 step with loss 0.628753125667572
training 700 step with loss 0.6419855952262878
training 800 step with loss 0.6378697156906128
training 900 step with loss 0.6406897306442261
training 1000 step with loss 0.6505377888679504
```

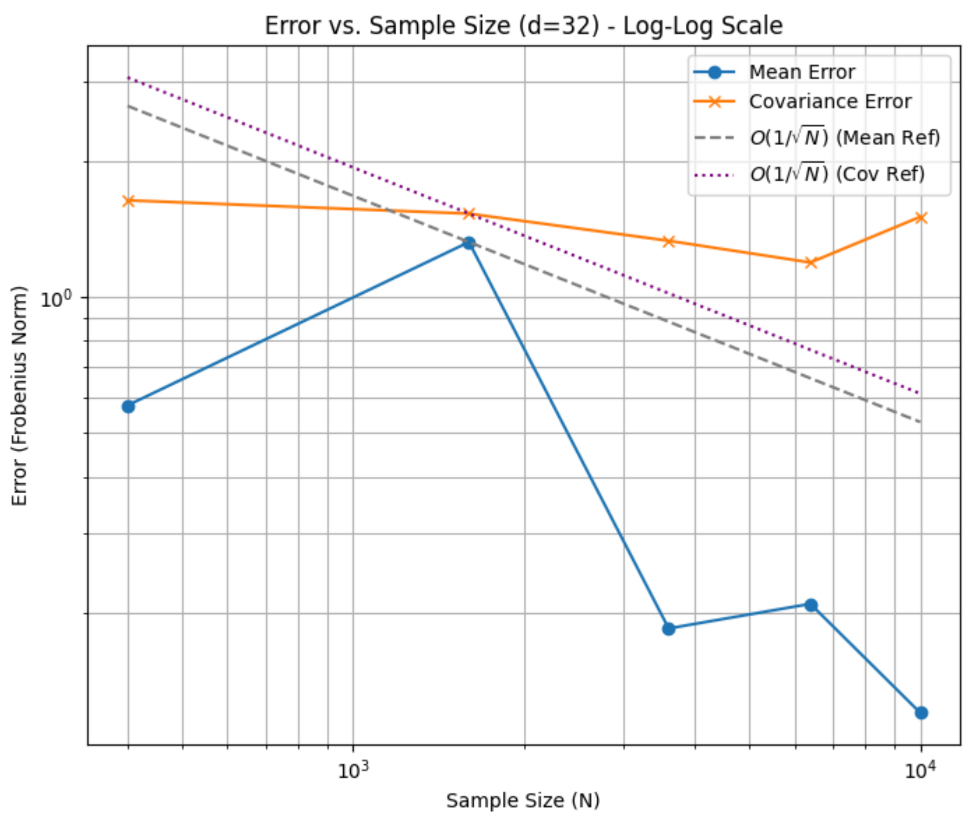
```
---------------------------------------------------------------------------
KeyboardInterrupt                         Traceback (most recent call last)
<ipython-input-25-e497deecf152> in <cell line: 0>()
     20 get_ipython().run_line_magic('store', 'N_experiment_64')
     21 
---> 22 mean_errors_128, cov_errors_128, N_experiment_128 = run_experiment_for_d(128, N_values,max_steps_per_logN=1500)
     23 get_ipython().run_line_magic('store', 'mean_errors_128')
     24 get_ipython().run_line_magic('store', 'cov_errors_128')

<ipython-input-23-36b2e0a927ae> in run_experiment_for_d(d, N_values, h, inf_h, t1, use_trained, max_steps_per_logN)
     42           # first pretrain on small batches
     43             # train(1000, 16, 0.005, t1 = 1, B  = 100, max_steps = 5000)
---> 44           model, xs = train_gpu(
     45               N, d, h, t1=t1,
     46               model=masked_p,

<ipython-input-19-2d947bebd717> in train_gpu(N, d, h, t1, B, model, epsilon, max_steps)
     21 
     22         optimizer.zero_grad()
---> 23         loss.backward()
     24 
     25         if(step%(min(max_steps//10, 100))==0):

/usr/local/lib/python3.11/dist-packages/torch/_tensor.py in backward(self, gradient, retain_graph, create_graph, inputs)
    624                 inputs=inputs,
    625             )
--> 626         torch.autograd.backward(
    627             self, gradient, retain_graph, create_graph, inputs=inputs
    628         )

/usr/local/lib/python3.11/dist-packages/torch/autograd/__init__.py in backward(tensors, grad_tensors, retain_graph, create_graph, grad
_variables, inputs)
    345     # some Python versions print out the first line of a multi-line function
    346     # calls in the traceback and some print out the last line
--> 347     _engine_run_backward(
    348         tensors,
    349         grad_tensors_,

/usr/local/lib/python3.11/dist-packages/torch/autograd/graph.py in _engine_run_backward(t_outputs, *args, **kwargs)
    821         unregister_hooks = _register_logging_hooks_on_whole_graph(t_outputs)
    822     try:
--> 823         return Variable._execution_engine.run_backward(  # Calls into the C++ engine to run the backward pass
    824             t_outputs, *args, **kwargs
    825         )  # Calls into the C++ engine to run the backward pass

KeyboardInterrupt: 
```

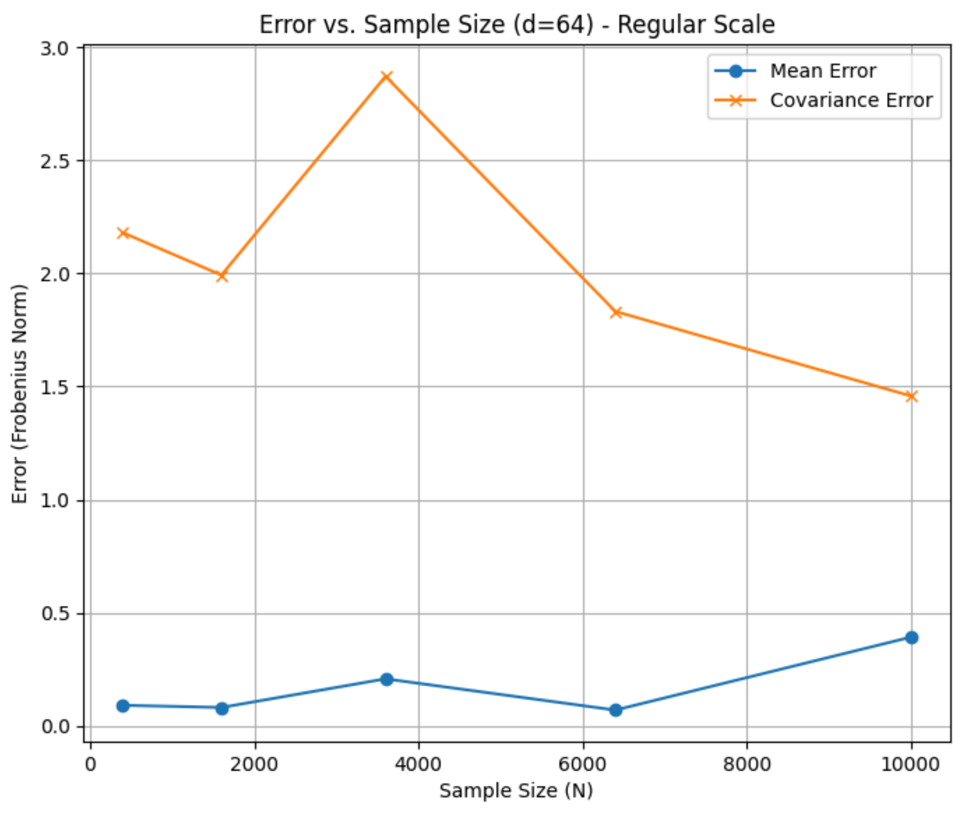
In [26]:

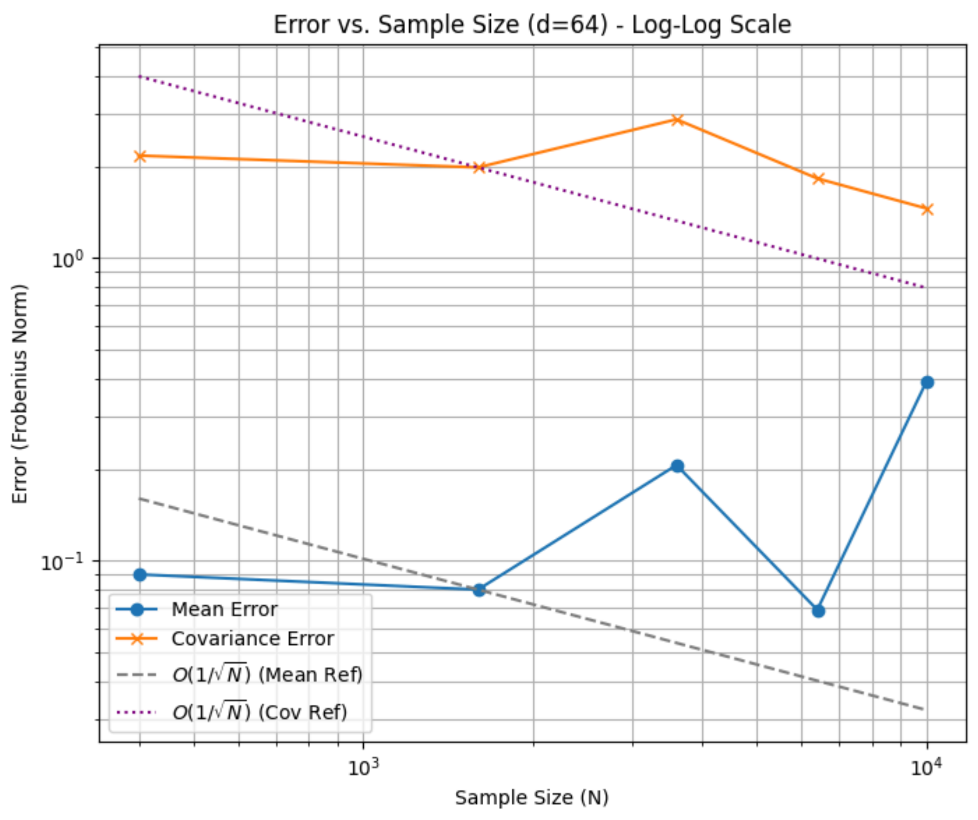
```python
# plot data
plot_errors(N_experiment_16, mean_errors_16, cov_errors_16, 16)
plot_errors(N_experiment_32, mean_errors_32, cov_errors_32, 32)
plot_errors(N_experiment_64, mean_errors_64, cov_errors_64, 64)
plot_errors(N_experiment_128, mean_errors_128, cov_errors_128, 128)
```











```
---------------------------------------------------------------------------
NameError                                 Traceback (most recent call last)
<ipython-input-26-382e5c026d2c> in <cell line: 0>()
      3 plot_errors(N_experiment_32, mean_errors_32, cov_errors_32, 32)
      4 plot_errors(N_experiment_64, mean_errors_64, cov_errors_64, 64)
----> 5 plot_errors(N_experiment_128, mean_errors_128, cov_errors_128, 128)

NameError: name 'N_experiment_128' is not defined
```

In the above examples for $d = 16, d = 32, d = 64$, we see a general trend of decreasing error both in covariance and in mean that is inversely proportional with the square root of sample size, $\frac{1}{\sqrt{N}}$. The match can be observed in the log log plot with a slope of $-\frac{1}{2}$, with the exception for d=64, where the mean was seen to be increasing. We have not yet found enough time to train the network for $d = 128$. With more time in training, we may find better convergence properties.