Phase 5 Epideimic Example

Our Target

In this project, we try to answer the question: In SIR model, given N (number of pupulation) and y_obs(number of infected people), what is the possible ditribution of the infection rate θ ?

We assume the prior of our infection rate to be Exponential with rate 1, and that since we do not know what is the realistic y_obs, we simulate it with our model sir_sim.

By obtaining our prior and y, we aim to approximate the posterior distribution $p(\theta|y,N)$ where:

- θ : infection rate parameter
- y: observed number of infections
- N: Household size

Model

We model this posterior based on data generated by a stochastic SIR household simulator. We compare two neural inference methods:

- Mixture Density Network (MDN)
- Conditional Normalising Flow (CNF)

Mixture Density Network(MDN), as we used before, is a combination of Gaussian distribution and Conditional Normalisin flow, is a flow that using sigmoid and affine transformation.

Step 1: Simulate the data

We simulate infection spread in a household using a simplified stochastic SIR process. For each household size N , we sample :

- $\theta \sim Exponential(1)$
- Run sir_sim(N, theta) to obtain a corresponding y.

Hence, We obtain tuples (θ, y, N) for training and evaluation. Where θ is our output, y and N being our input.

By choosing our N with $\{100,150,200,250,300\}$ with M (number of samples per N) = 100,000, we finally obtain the data with 500,000 rows and 3 columns.

We save the data using the code np.savetxt("theta_y_N_samples.txt", samples)

We are lucky because now we choose the rate of our prior to be 1, in which case the θ generated has limited maximum.

```
In [16]: # === ** Import Libraries ===
         import numpy as np
         import torch
         import torch.nn as nn
         import torch.optim as optim
         from torch.distributions import Normal
         from scipy.stats import norm
         import matplotlib.pyplot as plt
         from collections import defaultdict
         from tqdm import tqdm
         import os
         # === 🀙 SIR Simulator ===
         def sir_sim(N, lam, k=0):
             S = N - 1
             y = 1
             while y > 0:
                 y -= 1
                 I = 1.0 if k == 0 else np.random.gamma(shape=k, scale=1/k)
                 Z = np.random.poisson(lam * I)
                 for in range(Z):
                     if np.random.rand() < S / N:</pre>
                         S -= 1
                         y += 1
             return N - S - 1
         # === II Generate Samples ===
         def generate_theta_y_N_samples(M_per_N=100000, N_list=[100, 200, 300], prior
             all_samples = []
             for N in N list:
                 for _ in tqdm(range(M_per_N), desc=f"Generating samples for N={N}"):
                     theta = np.random.exponential(scale=1 / prior rate)
                     y = sir sim(N, lam=theta, k=0)
                     all samples.append([theta, y, N])
             return np.array(all_samples)
         # === 🗹 Generate + Save ===
         N list = [100,150, 200,250, 300]
         samples = generate_theta_y_N_samples(M_per_N=100000, N_list=N_list)
         np.savetxt("theta y N samples.txt", samples)
         # === 📥 Load + Normalize ===
         data = np.loadtxt("theta y N samples.txt")
         theta_all, y_all, N_all = data[:, 0], data[:, 1].astype(int), data[:, 2].ast
         y max, N max = int(y all.max()), int(N all.max())
         x_max = 5.0
         pair dict = defaultdict(list)
```

```
for theta_val, y_val, N_val in zip(theta_all, y_all, N_all):
    pair_dict[(y_val, N_val)].append(theta_val)

def normalize_y_N(y, N, y_max, N_max):
    return y / y_max, N / N_max
```

```
Generating samples for N=100: 100\% | 100000/100000 [00:01<00:00, 5 0695.72it/s] Generating samples for N=150: 100\% | 100000/100000 [00:02<00:00, 3 7546.81it/s] Generating samples for N=200: 100\% | 100000/100000 [00:03<00:00, 2 8956.20it/s] Generating samples for N=250: 100\% | 100000/100000 [00:04<00:00, 2 1645.53it/s] Generating samples for N=300: 100\% | 100000/100000 [00:05<00:00, 1 9552.40it/s]
```

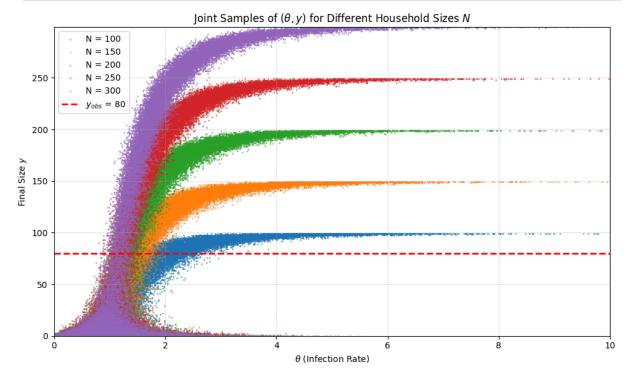
We can see from the output that for each N = 100, N = 200, N = 300 ,we genetate 100000 rows for each. It is also worth noting that more time is needed to generate for big N, because for large θ , it would take longer time to infect all the population.

Visualisation on Different N

Acutally, we can plot how our y_obs varies for different θ under differen N. We wonder if our two models could sufficiently capture the distribution under different N, so a plot of all the data points is necessary.

```
In [17]: import matplotlib.pyplot as plt
         # Choose which N values to plot
         N values to plot = [100,150, 200,250, 300] # You can modify this list
         plt.figure(figsize=(10, 6))
         for N_target in N_values_to_plot:
             # Mask data for current N
             mask = N all == N target
             theta_subset = theta_all[mask]
             y_subset = y_all[mask]
             plt.scatter(theta_subset, y_subset, s=1, alpha=0.5, label=f"N = {N_targe
         # Optional: draw a horizontal line at a specific y obs
         y obs = 80
         plt.axhline(y=y_obs, color='red', linestyle='--', linewidth=2, label=r"$y_{color='red'}
         # Plot settings
         plt.xlabel(r"$\theta$ (Infection Rate)")
         plt.ylabel("Final Size $y$")
         plt.title("Joint Samples of $(\\theta, y)$ for Different Household Sizes $N$
         plt.legend()
         plt.grid(True, alpha=0.3)
         plt.xlim(0, 10)
```

```
plt.ylim(0, max(y_all))
plt.tight_layout()
plt.show()
```



See the normalized y/N

To make the outbreak sizes comparable across different household sizes N, we normalized the final size y by dividing it by N.

This normalization allows us to interpret the outcome as a proportion of the total population that was infected.

However, visualizing $(\theta, y/N)$ jointly for multiple N values on the same scatter plot can lead to heavy overlap, which is hard for our NN to capture the features.

In contrast, the unnormalized plot (using (y)) separates different (N) values vertically, making the scatter less dense but also less comparable in terms of proportion. For better visual clarity, alternative methods such as contour plots, hexbin plots, or separate subplots for each (N) may be used.

```
import matplotlib.pyplot as plt

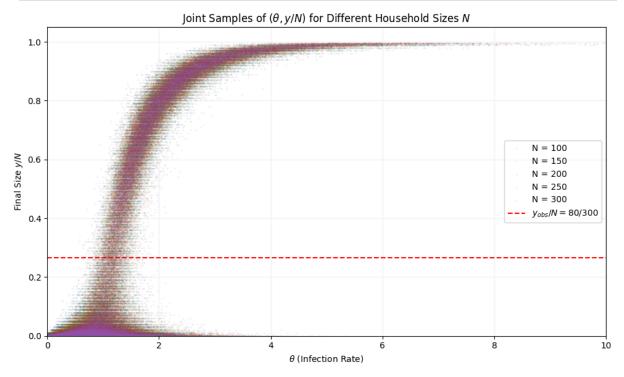
# Choose which N values to include
N_values_to_plot = [100,150, 200,250, 300] # or list(set(N_all)) for all un

plt.figure(figsize=(10, 6))

for N_target in N_values_to_plot:
    mask = N_all == N_target
    theta_subset = theta_all[mask]
```

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```
y_subset = y_all[mask]
   y_normalized = y_subset / N_target # Normalize y by N
   plt.scatter(theta_subset, y_normalized, s=1, alpha=0.05, label=f"N = {N_
# Optional: draw horizontal line for a reference normalized y_obs
y obs = 80
plt.axhline(y=y_obs / max(N_values_to_plot), color='red', linestyle='--', la
# Labels and title
plt.xlabel(r"$\theta$ (Infection Rate)")
plt.ylabel(r"Final Size $y/N$")
plt.title("Joint Samples of $(\\theta, y/N)$ for Different Household Sizes $
plt.legend()
plt.grid(True, alpha=0.1)
plt.xlim(0, 10)
plt.ylim(0, 1.05)
plt.tight layout()
plt.show()
```



The red dashed line represents a reference observation $y_{obs}/N=80/300\approx0.267$.

While admitting that some subtle differences between different N exist and may be captured by our NN, almost all points collapse into a similar region after normalization.

In this case, the idea that using y/N as our input is not a great idea.

Model 1: Normalising Flow

We implement a 1D conditional affine flow:

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- Inputs: $x = \theta \in (0, 1)$ (after sigmoid transformation)
- Condition: normalized (y, N)
- Composed of: affine + sigmoid transformation layers
- Base distribution: standard Normal

Loss:

$$\mathcal{L}_{ ext{Flow}} = -\log p_{ ext{base}}(z) - \log \left| rac{dz}{dx}
ight|$$

Hyperparameters:

- Epochs: 300
- Optimizer: Adam (lr = 1e-3)
- Loss: $-\log(p(\theta|y, N))$ via change of variables
- Hidden Layes: 3 layers with 64 units each
- Number of flow: 1

```
In [ ]: base_dist = Normal(loc=0.0, scale=1.0)
        class ConditionalAffineFlow(nn.Module):
            def __init__(self, cond_dim, hidden_dim=128):
                super().__init__()
                self.net = nn.Sequential(
                    nn.Linear(cond_dim, hidden_dim), nn.ReLU(),
                    nn.Linear(hidden_dim, hidden_dim), nn.ReLU(),
                    nn.Linear(hidden dim, hidden dim), nn.ReLU(),
                    nn.Linear(hidden dim, 2) # scale and shift
                )
            def forward(self, z, cond):
                cond_out = self.net(cond)
                scale = cond out[:, 0:1]
                shift = cond out[:, 1:2]
                u = torch.exp(scale) * z + shift
                x = torch.sigmoid(u)
                \log_{det} = scale + torch.log(x * (1 - x) + 1e-6)
                return x, log_det
            def inverse(self, x, cond):
                cond_out = self.net(cond)
                scale = cond_out[:, 0:1]
                shift = cond_out[:, 1:2]
                u = torch.log(x) - torch.log1p(-x)
                z = (u - shift) / torch.exp(scale)
                log_det = -scale - torch.log(x * (1 - x) + 1e-6)
                return z, log_det
        class ConditionalNormalizingFlow1D(nn.Module):
            def __init__(self, cond_dim, num_layers=1):
                super(). init ()
                self.layers = nn.ModuleList([ConditionalAffineFlow(cond_dim) for _ i
```

```
def forward(self, x, cond):
                 z, log det = x, torch_zeros like(x)
                 for layer in reversed(self.layers):
                     z, ldj = layer.inverse(z, cond)
                     log det += ldj
                 return base_dist.log_prob(z) + log_det
             def sample(self, cond, n samples=100):
                 z = base dist.sample((n samples, 1))
                 cond = cond.expand(n_samples, -1)
                 for layer in self.layers:
                     x, _ = layer.forward(x, cond)
                 return x
In [24]: flow = ConditionalNormalizingFlow1D(cond dim=2, num layers=1)
         optimizer = optim.Adam(flow.parameters(), lr=1e-3)
         n = 500
         losses = []
         for epoch in tgdm(range(n epochs), desc="Training Flow"):
             total_loss = 0.0
             count = 0
             for (y_val, N_val), theta_vals in pair_dict.items():
                 if len(theta vals) < 50:</pre>
                     continue
                 x = torch.tensor(theta vals, dtype=torch.float32).unsqueeze(1)
                 x = (x / x_max).clamp(1e-4, 1 - 1e-4)
                 y_norm, N_norm = normalize_y_N(y_val, N_val, y_max, N_max)
                 cond = torch.tensor([[y_norm, N_norm]], dtype=torch.float32).repeat(
                 log prob = flow(x, cond)
                 loss = -log prob.mean()
                 optimizer.zero_grad()
                 loss.backward()
                 optimizer.step()
                 total_loss += loss.item()
                 count += 1
             losses.append(total_loss / max(count, 1))
             if epoch % 10 == 0:
                 print(f"Epoch {epoch}: Loss = {losses[-1]:.4f}")
         torch.save(flow.state_dict(), "flow_model_multiN.pth")
        Training Flow:
                                       | 1/500 [00:01<10:18, 1.24s/it]
        Epoch 0: Loss = -0.1895
        Training Flow: 2%||
                                      | 11/500 [00:08<05:59, 1.36it/s]
        Epoch 10: Loss = -1.2988
        Training Flow:
                                      21/500 [00:16<06:15, 1.28it/s]
                         4%||
```

```
file:///Users/zhangying/Documents/Research/Bayesian/Code/Week 7/Flow_MOG_report.html
```

Epoch 20: Loss = -1.6606

Training Flow:		31/500 [00:23<05:30, 1.42it/s]
Epoch 30: Loss = Training Flow:		41/500 [00:30<05:10, 1.48it/s]
Epoch 40: Loss = Training Flow:		51/500 [00:37<05:02, 1.48it/s]
Epoch 50: Loss =	= -1.8006	
Training Flow: Epoch 60: Loss =	= -1.7998	61/500 [00:44<05:02, 1.45it/s]
Training Flow: Epoch 70: Loss =		71/500 [00:50<04:50, 1.48it/s]
Training Flow: Epoch 80: Loss =		81/500 [00:57<04:58, 1.40it/s]
Training Flow: Epoch 90: Loss =	18%	91/500 [01:04<04:22, 1.56it/s]
Training Flow: Epoch 100: Loss		101/500 [01:10<04:31, 1.47it/s]
Training Flow: Epoch 110: Loss		111/500 [01:17<04:29, 1.44it/s]
Training Flow:	24%	121/500 [01:24<04:17, 1.47it/s]
Epoch 120: Loss Training Flow:	26%	131/500 [01:31<04:02, 1.52it/s]
Epoch 130: Loss Training Flow:		141/500 [01:37<03:58, 1.50it/s]
Epoch 140: Loss Training Flow:		151/500 [01:44<03:50, 1.51it/s]
Epoch 150: Loss	= -1.8034	
Training Flow: Epoch 160: Loss	·	161/500 [01:50<03:35, 1.58it/s]
Training Flow: Epoch 170: Loss		171/500 [01:57<03:28, 1.58it/s]
Training Flow: Epoch 180: Loss		181/500 [02:03<03:21, 1.58it/s]
Training Flow: Epoch 190: Loss	38%	191/500 [02:09<03:14, 1.59it/s]
Training Flow:	40%	201/500 [02:17<03:32, 1.41it/s]
Epoch 200: Loss Training Flow:		211/500 [02:24<03:27, 1.40it/s]
Epoch 210: Loss Training Flow:		221/500 [02:32<03:42, 1.26it/s]
Epoch 220: Loss	= -1.8338	
Training Flow: Epoch 230: Loss		231/500 [02:39<03:14, 1.38it/s]
Training Flow: Epoch 240: Loss	48% 338	241/500 [02:47<03:23, 1.27it/s]
Training Flow: Epoch 250: Loss	50%	251/500 [02:55<03:01, 1.37it/s]
Training Flow:	52%	261/500 [03:03<03:20, 1.19it/s]
Epoch 260: Loss Training Flow:	= -1.8410 54%	271/500 [03:11<03:12, 1.19it/s]

```
Epoch 270: Loss = -1.8369
                            | 281/500 [03:18<02:28, 1.47it/s]
Training Flow: 56%
Epoch 280: Loss = -1.8335
Training Flow: 58%
                            | 291/500 [03:25<02:33, 1.36it/s]
Epoch 290: Loss = -1.8390
Training Flow: 60%
                            | 301/500 [03:32<02:20, 1.41it/s]
Epoch 300: Loss = -1.8433
Training Flow: 62%
                            | 311/500 [03:39<02:09, 1.46it/s]
Epoch 310: Loss = -1.8448
Training Flow: 64%
                            | 321/500 [03:46<02:03, 1.44it/s]
Epoch 320: Loss = -1.8429
                            | 331/500 [03:53<01:57, 1.43it/s]
Training Flow: 66%
Epoch 330: Loss = -1.8333
Training Flow: 68%
                            | 341/500 [04:00<01:45, 1.50it/s]
Epoch 340: Loss = -1.8269
Training Flow: 70%
                            | 351/500 [04:06<01:43, 1.44it/s]
Epoch 350: Loss = -1.8494
Training Flow: 72%
                            | 361/500 [04:13<01:34, 1.47it/s]
Epoch 360: Loss = -1.8289
Training Flow: 74%
                            | 371/500 [04:20<01:35, 1.35it/s]
Epoch 370: Loss = -1.7357
Training Flow: 76%
                            | 381/500 [04:28<01:22, 1.45it/s]
Epoch 380: Loss = -1.8383
Training Flow: 78%
                            | 391/500 [04:34<01:17, 1.41it/s]
Epoch 390: Loss = -1.8506
Training Flow: 80%
                           | 401/500 [04:41<01:06, 1.50it/s]
Epoch 400: Loss = -1.8438
Training Flow: 82%
                           | 411/500 [04:48<01:01, 1.46it/s]
Epoch 410: Loss = -1.8464
Training Flow: 84% 421/500 [04:55<00:58, 1.35it/s]
Epoch 420: Loss = -1.8513
Training Flow: 86%
                        431/500 [05:02<00:44, 1.54it/s]
Epoch 430: Loss = -1.7260
Training Flow: 88%
                         441/500 [05:09<00:38, 1.55it/s]
Epoch 440: Loss = -1.8398
Training Flow: 90% 451/500 [05:15<00:31, 1.55it/s]
Epoch 450: Loss = -1.8139
                          | | 461/500 [05:22<00:25,
                                                  1.53it/s]
Training Flow: 92%
Epoch 460: Loss = -1.8474
Training Flow: 94% 471/500 [05:28<00:18, 1.57it/s]
Epoch 470: Loss = -1.8402
Training Flow: 96%
                          | 481/500 [05:35<00:12, 1.53it/s]
Epoch 480: Loss = -1.8450
Training Flow: 98% 491/500 [05:41<00:05, 1.56it/s]
Epoch 490: Loss = -1.8517
Training Flow: 100%| 500/500 [05:47<00:00,
                                                  1.44it/sl
```

Model 2: Mixture Density Network

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We can also use mixture density network to fit our training dataset.

- Input: $[N/N_{\rm max},\ y/y_{\rm max}]$, normalized
- Output: K Gaussian components (weights π , means μ)

In our MDG model, it gives a 3-layer feedforward network outputs:

- $\pi_k(y, N)$: mixture weights (softmax)
- $\mu_k(y,N)$: means of Gaussians
- $\sigma_k^2(y,N)$: variances (via log-variance output)

with a **Loss** of

$$\mathcal{L}_{ ext{MDN}} = -\mathbb{E}_{ heta} \left[\log \sum_{k} \pi_k \cdot \mathcal{N}(heta \mid \mu_k, \sigma_k^2)
ight]$$

Hyperparameters:

- Epochs: 300
- Optimizer: Adam (lr = 1e-3)
- Loss: $-\log(p(\theta|y, N))$ via change of variables
- Hidden layers: Three layers with 64 units.
- Components: The number of components is K = 3

The code below defines the structure of our MDN model.

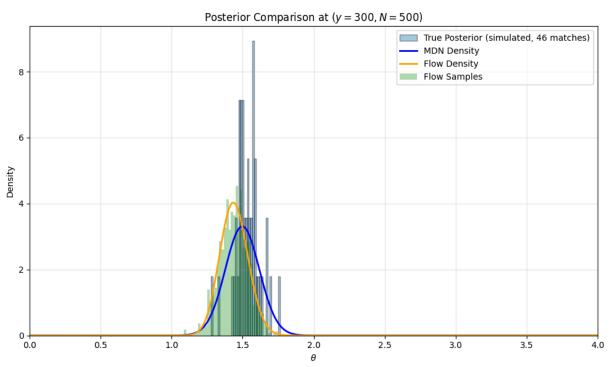
```
In [31]: class MixtureDensityNN MultiN(nn.Module):
             def __init__(self, input_dim=2, hidden_dim=128, K=3):
                 super().__init__()
                  self.K = K
                  self.hidden = nn.Sequential(
                      nn.Linear(input_dim, hidden_dim), nn.Tanh(),
                     nn.Linear(hidden_dim, hidden_dim), nn.Tanh(),
                     nn.Linear(hidden_dim, hidden_dim), nn.Tanh()
                  self.pi layer = nn.Linear(hidden dim, K)
                  self.mu layer = nn.Linear(hidden dim, K)
                  self.log_var_layer = nn.Linear(hidden_dim, K)
             def forward(self, x):
                 h = self.hidden(x)
                 pi = torch.softmax(self.pi layer(h), dim=1)
                 mu = self.mu layer(h)
                  log_var = self.log_var_layer(h).clamp(min=-10, max=10)
                  return pi, mu, log var
         def mixture_log_likelihood(theta_vals, weights, mu, log_var):
             var = torch.exp(log_var)
             theta = theta vals.expand(-1, mu.shape[1])
             \log_{probs} = -0.5 * (\log_{var} + np.\log(2 * np.pi) + (theta - mu)**2 / var)
             log_weighted = torch.log(weights + 1e-8) + log_probs
```

```
return -torch.logsumexp(log weighted, dim=1).mean()
 def train multi N mdn(data, K=5, hidden dim=128, n epochs=500):
     theta_all, y_all, N_all = data[:, 0], data[:, 1].astype(int), data[:, 2]
     pair_dict = defaultdict(list)
     for theta, y, N in zip(theta_all, y_all, N_all):
         pair_dict[(N, y)].append(theta)
     N \max = \max(N \text{ all})
     y_max = max(y_all)
     model = MixtureDensityNN MultiN(input dim=2, hidden dim=hidden dim, K=K)
     optimizer = optim.Adam(model.parameters(), lr=1e-3)
     for epoch in range(n epochs):
         model.train()
         total_loss = 0.0
         count = 0
         for (N_val, y_val), theta_list in pair_dict.items():
             if len(theta_list) < 5:</pre>
                 continue
             x_input = torch.tensor([[N_val / N_max, y_val / y_max]], dtype=t
             theta_vals = torch.tensor(theta_list, dtype=torch.float32).view(
             pi, mu, log var = model(x input)
             loss = mixture log likelihood(theta vals, pi, mu, log var)
             optimizer.zero_grad()
             loss.backward()
             optimizer.step()
             total_loss += loss.item()
             count += 1
         if epoch % 50 == 0:
             print(f"Epoch {epoch}, Loss: {total loss / max(count, 1):.5f}")
     return model, N_max, y_max
 # === / Train MDN ===
 model, N_max, y_max = train_multi_N_mdn(data, K=5, hidden_dim=64, n_epochs=5
 os.makedirs("saved_model", exist_ok=True)
 torch.save(model.state dict(), "saved model/mdn multiN.pth")
 np.savez("saved_model/meta.npz", N_max=N_max, y_max=y_max)
Epoch 0, Loss: 0.20269
Epoch 50, Loss: -0.25101
Epoch 100, Loss: -0.26078
Epoch 150, Loss: -0.26636
Epoch 200, Loss: -0.26565
Epoch 250, Loss: -0.27316
Epoch 300, Loss: -0.27584
Epoch 350, Loss: -0.27917
Epoch 400, Loss: -0.27343
Epoch 450, Loss: -0.27409
```

Visualization

```
In [46]: def compare mdn and flow(mdn model, flow model, y obs, N obs, N max, y max,
             y_norm, N_norm = y_obs / y_max, N_obs / N_max
             cond tensor = torch.tensor([[N norm, y norm]], dtype=torch.float32)
             flow cond = torch.tensor([[y norm, N norm]], dtype=torch.float32)
             theta sampled flow = flow model.sample(flow cond, n samples=1000).detach
             theta grid = torch.linspace(1e-4, 1 - 1e-4, 500).unsqueeze(1)
             cond grid = flow cond.expand(theta grid.shape[0], 2)
             with torch.no_grad():
                 log prob = flow model(theta grid, cond grid)
                 flow_density = (torch.exp(log_prob) / x_max).numpy().flatten()
             theta_grid_real = (theta_grid * x_max).numpy().flatten()
             with torch.no grad():
                 pi, mu, log_var = mdn_model(cond_tensor)
             pi = pi.numpy().flatten()
             mu = mu.numpy().flatten()
             sigma = np.sqrt(np.exp(log_var.numpy().flatten()))
             mdn density = sum(pi[k] * norm.pdf(theta grid real, mu[k], sigma[k]) for
             key = (y_obs, N_obs)
             if key in pair dict:
                 true_theta_vals = np.array(pair_dict[key])
                 label gt = "True Posterior (from training)"
             elif simulate ground truth:
                 theta vals, y vals = [], []
                 for _ in range(M):
                     theta = np.random.exponential(scale=1.0)
                     y = sir_sim(N_obs, lam=theta)
                     theta_vals.append(theta)
                     y_vals.append(y)
                 true theta vals = np.array([t for t, y in zip(theta vals, y vals) if
                 label_gt = f"True Posterior (simulated, {len(true_theta_vals)} match
             else:
                 true theta vals = None
                 label_gt = None
             plt.figure(figsize=(10, 6))
             if true_theta_vals is not None and len(true_theta_vals) > 0:
                 plt.hist(true_theta_vals, bins=40, density=True, alpha=0.4, label=la
             plt.plot(theta_grid_real, mdn_density, lw=2, label="MDN Density", color=
             plt.plot(theta_grid_real, flow_density, lw=2, label="Flow Density", cold
             plt.hist(theta_sampled_flow, bins=40, density=True, alpha=0.3, label="Fl
             plt.xlabel(r"$\theta$")
             plt.xlim(0, 4)
             plt.ylabel("Density")
             plt.title(rf"Posterior Comparison at $(y={y obs}, N={N obs})$")
             plt.legend()
             plt.grid(True, alpha=0.3)
             plt.tight layout()
             plt.show()
```

```
compare_mdn_and_flow(
    mdn_model=model,
    flow_model=flow,
    y_obs=300,
    N_obs=500,
    N_max=N_max,
    y_max=y_max,
    x_max=x_max,
    pair_dict=pair_dict,
    simulate_ground_truth=True
)
```



Interpretation of the result

In this setting, we observe for multiple different pairs of y and N, so for N seen in the training dataset, like N = 100, 200, 300, both models perform well.

And for N unseen, we generate the data again and then compare. For now, the MDN is performing better than normalising flow for same architecture.

Conclusion: Both MDN and Flow demonstrate reasonable generalization to unseen (N), with MDN producing slightly smoother densities. This supports the potential of neural posterior approximators in amortized likelihood-free inference.

```
In []:
In []:
```