Phase 4

Learning posterior via Normalising Flow for Beta-Binomial model Ying & Danny
Date: 2025-07-08

Beta as Toy Example

A Glimpse of our example

Now assume our posterior is hard to find (though in this toy example it is tractable).

- **Prior:**

$$\theta \sim \mathrm{Beta}(\alpha, \beta)$$

- **Likelihood:**
  For each experiment $i = 1, \ldots, N$,

$$y_i \sim \mathrm{Binomial}(n, \theta),$$

  and let

$$\Sigma_y = \sum_{i=1}^{N} y_i.$$

By conjugacy, the true posterior is

$$\theta \mid \{y_i\} \sim \mathrm{Beta}\big(\alpha + \Sigma_y,\ \beta + N\,n - \Sigma_y\big).$$

Example parameters:

$$\alpha = 2, \quad \beta = 5, \quad N = 3, \quad n = 11, \quad \Sigma_y = 15.$$

Hence the posterior becomes

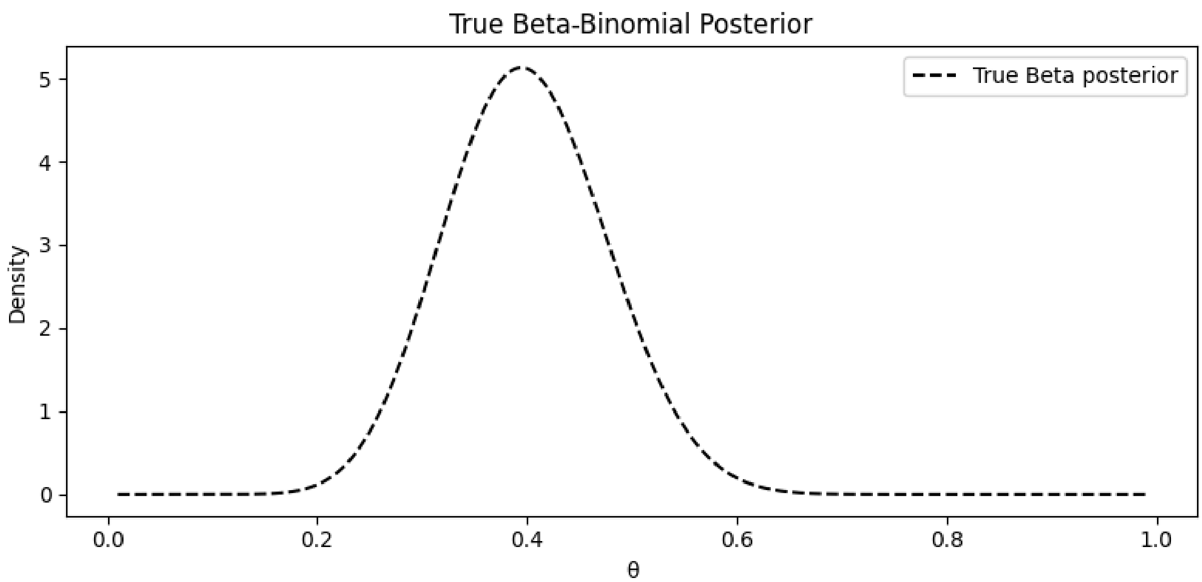
$$\theta \mid \{y_i\} \sim \mathrm{Beta}\big(2 + 15,\ 5 + 3 \cdot 11 - 15\big) = \mathrm{Beta}(17,\ 23).$$

The plot of the true Beta posterior is given below.

Check that the posterior mean is

$$\mathbb{E}[\theta] = \frac{\alpha + \Sigma_y}{\alpha + \beta + N\,n} = \frac{17}{17 + 23} = \frac{17}{40} \approx 0.425.$$

In [9]:
```
import torch
import numpy as np
import matplotlib.pyplot as plt
from scipy.stats import beta as beta_dist

def plot_true_posterior(x_grid, alpha_post, beta_post):
    true_pdf = beta_dist.pdf(x_grid, a=alpha_post, b=beta_post)

    plt.figure(figsize=(8, 4))
    plt.plot(x_grid, true_pdf, '--', label='True Beta posterior', color='bla
    plt.xlabel('θ')
    plt.ylabel('Density')
    plt.title('True Beta-Binomial Posterior')
    plt.legend()
    plt.tight_layout()
    plt.show()

# Parameters and data
all_y_obs = torch.tensor([7., 3., 4., 6., 2., 8., 5., 1., 9., 10.])  # pool
n_trials = 11
alpha0, beta0 = 2.0, 5.0
x = np.linspace(0.01, 0.99, 500)

# Use N = 3
N = 3
y_obs = all_y_obs[:N]
sum_y = y_obs.sum()
alpha_post = alpha0 + sum_y
beta_post = beta0 + N * n_trials - sum_y

#  true posterior
plot_true_posterior(x_grid=x, alpha_post=alpha_post.item(), beta_post=beta_p
```



Our target

We want to check whether NF has equivalently expressive power as the true posterior. In this case , we assume a normalising flow from a standard normal distribution would well fit the posterior, who is simply an affine transformation and a sigmoid function.

Evaluating method: KL-Divergence

We assume our our normalising flow gives us the transformed distribution $q(\theta|y)$ So We now use KL-divergence to represent the distance between the true posterior and our estimated posterior.

$$\mathrm{KL}(q_\phi(\theta \mid \mathbf{y}) \,\|\, \pi(\theta \mid \mathbf{y})) = \mathbb{E}_{q_\phi(\theta|\mathbf{y})}\left[\log \frac{q_\phi(\theta \mid \mathbf{y})}{\pi(\theta \mid \mathbf{y})}\right]$$

And based on Beyesian theorem, we have:

$$\pi(\theta \mid \mathbf{y}) \propto \pi(\mathbf{y} \mid \theta)\pi(\theta)$$

Plugging into the KL expression:

$$\mathrm{KL}(q_\phi \,\|\, \pi) = \mathbb{E}_{q_\phi}\left[\log q_\phi(\theta \mid \mathbf{y}) - \log \pi(\mathbf{y} \mid \theta) - \log \pi(\theta) + \log \pi(\mathbf{y})\right] \tag{1}$$

Since $\pi(\mathbf{y})$ is constant with respect to θ, it can be dropped when optimizing:

$$\mathrm{KL}(q_\phi \,\|\, \pi) = \mathbb{E}_{q_\phi}\left[\log q_\phi(\theta \mid \mathbf{y}) - \log \pi(\mathbf{y} \mid \theta) - \log \pi(\theta)\right] + \mathrm{const} \tag{2}$$

Thus, our variational objective (negative ELBO) is defined as:

$$\mathcal{L}(\phi) = \mathbb{E}_{q_\phi}\left[\log q_\phi(\theta \mid \mathbf{y}) - \log \pi(\mathbf{y} \mid \theta) - \log \pi(\theta)\right] \tag{3}$$

Minimizing $\mathcal{L}(\phi)$ is equivalent to minimizing the KL divergence between the variational approximation and the true posterior.

Training Principle

We define the training loss as:

$$\mathcal{L}(\phi) = \log q_\phi(\theta \mid y) - \log \pi(y \mid \theta) - \log \pi(\theta).$$

This requires computing:

1. **Log-prior**

```
log_prior = Beta(alpha0, beta0).log_prob(theta)
```

```
log_lik = Binomial(n_trials, theta_rep).log_prob(y_rep).sum(dim=1)
```

Flow density via change-of-variables:

$$\log q_\phi(\theta \mid y) = \log q(z) - \log\left|\frac{d\theta}{dz}\right| = \log q(z) - \log|a| - \log\big(\theta(1-\theta)\big).$$

We implement:

```
log_q = log_qz - torch.log(scale) - torch.log(theta * (1 - theta))
```

Start Training

We define the basic affine transformation as `shift` and `scale`, and the transformed theta would also experience a sigmoid function then our log_q and theta is put into the loss function.

In [10]:
```python
import torch
import torch.nn as nn
import torch.optim as optim
import matplotlib.pyplot as plt
from scipy.stats import beta as beta_dist
import numpy as np
from tqdm import trange
torch.manual_seed(0)
```

Out[10]: <torch._C.Generator at 0x118afc5f0>

In [11]:
```python
# -------- Base class for Flow --------
class BaseFlow(nn.Module):
    def __init__(self):
        super().__init__()

    def sample(self, batch_size, y_obs):
        raise NotImplementedError

    def eval_log_prob(self, x_grid, y_obs):
        raise NotImplementedError

# -------- Affine Flow in Logit Space --------
class AffineFlowLogit(BaseFlow):
    def __init__(self, obs_dim):
        super().__init__()
        self.linear = nn.Linear(obs_dim, 2)

    def _get_params(self, y_obs):
        params = self.linear(y_obs.unsqueeze(0))  # (1, 2)
        log_scale = params[0, 0]
        shift = params[0, 1]
        scale = torch.exp(log_scale)
        return scale, shift

    def sample(self, batch_size, y_obs):
        z = torch.randn(batch_size)
        scale, shift = self._get_params(y_obs)
        logit_theta = scale * z + shift
        theta = torch.sigmoid(logit_theta).clamp(1e-6, 1 - 1e-6)

        log_qz = torch.distributions.Normal(0, 1).log_prob(z)
        log_jacobian = torch.log(theta * (1 - theta))
        log_q = log_qz - torch.log(scale) - log_jacobian
```

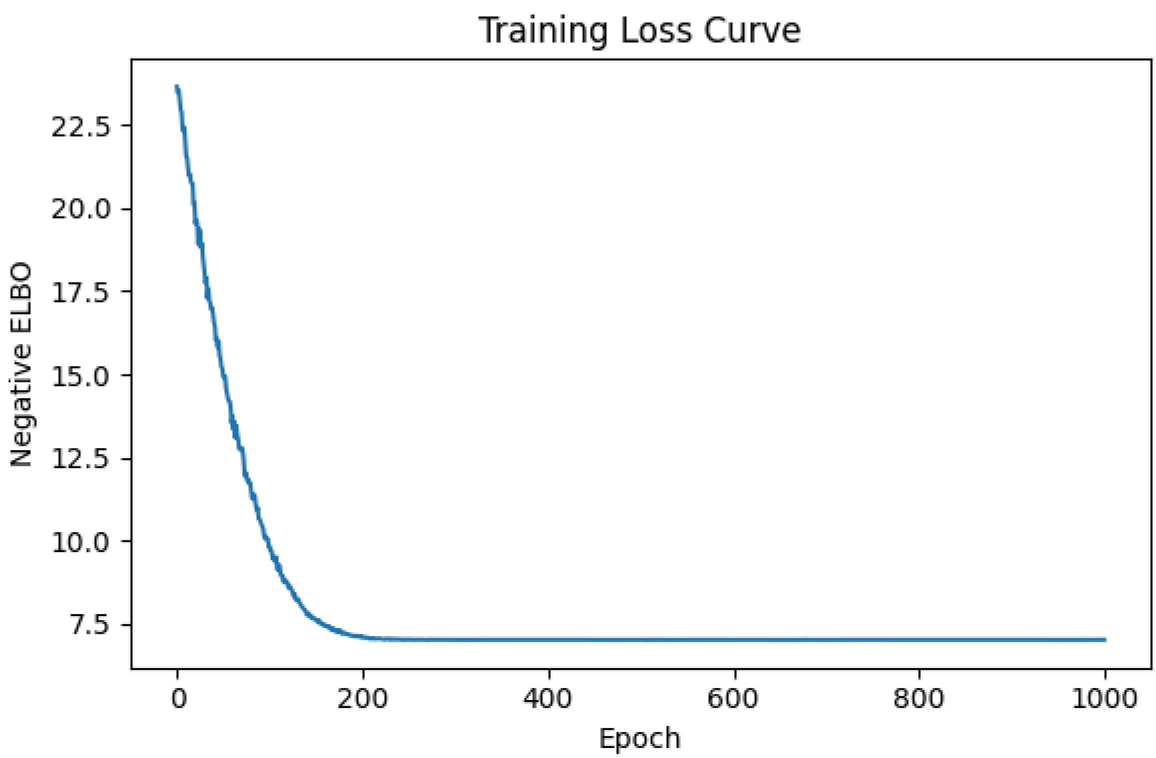
```python
        return theta, log_q

    def eval_log_prob(self, x_grid, y_obs):
        scale, shift = self._get_params(y_obs)
        x_t = torch.tensor(x_grid)
        logit_x = torch.log(x_t / (1 - x_t))
        z_x = (logit_x - shift) / scale
        log_qz = torch.distributions.Normal(0, 1).log_prob(z_x)
        log_qx = log_qz - torch.log(scale) - torch.log(x_t * (1 - x_t))
        return log_qx.exp().detach().numpy()
```

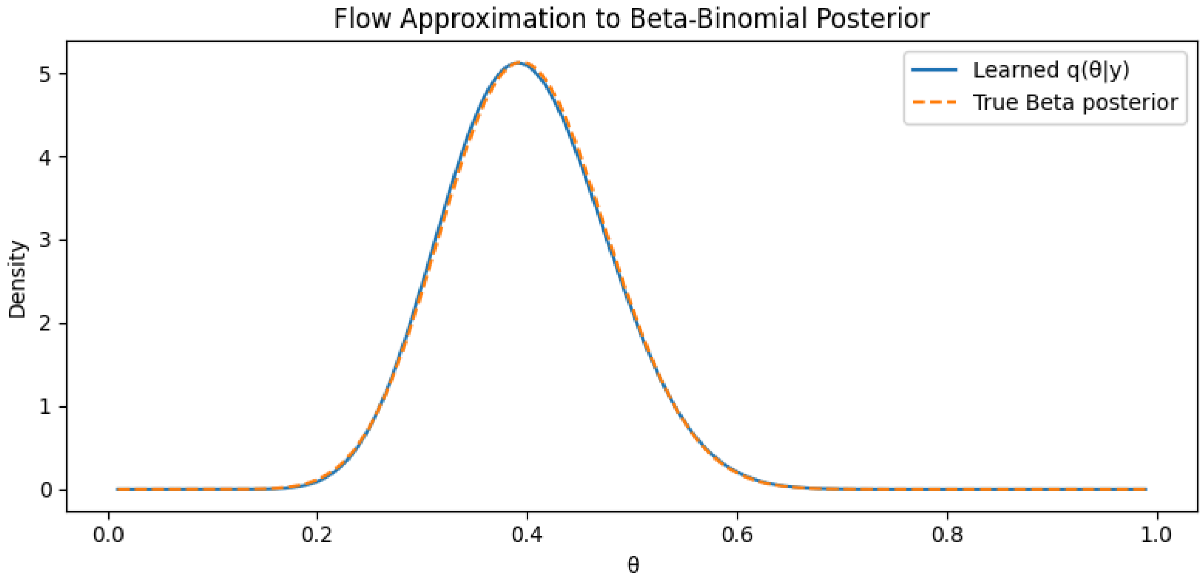
In [12]:
```python
# -------- Training Function --------
def train_flow(flow, y_obs, alpha0, beta0, n_trials, n_epochs=1000, n_sample
    optimizer = optim.Adam(flow.parameters(), lr=lr)
    N = y_obs.shape[0]
    losses = []
    for epoch in trange(n_epochs,desc="Training Flow"):
        optimizer.zero_grad()
        theta, log_q = flow.sample(n_samples, y_obs)
        # Prior: Beta(α0, β0)
        log_prior = torch.distributions.Beta(alpha0, beta0).log_prob(theta)
        # Likelihood: product of Binomial(n_trials, θ_i)
        theta_rep = theta.unsqueeze(1).expand(-1, N)
        y_rep = y_obs.unsqueeze(0).expand_as(theta_rep)
        log_lik = torch.distributions.Binomial(n_trials, theta_rep).log_prob
        # ELBO
        elbo = (log_prior + log_lik - log_q).mean()
        loss = -elbo
        loss.backward()
        optimizer.step()
        losses.append(loss.item())
    plt.figure(figsize=(6, 4))
    plt.plot(losses)
    plt.xlabel("Epoch")
    plt.ylabel("Negative ELBO")
    plt.title("Training Loss Curve")
    plt.tight_layout()
    plt.show()
    return losses
```

In [13]:
```python
# -------- Plotting Function --------
def plot_density(flow, y_obs, x_grid, alpha_post, beta_post):
    q_pdf = flow.eval_log_prob(x_grid, y_obs)
    true_pdf = beta_dist.pdf(x_grid, a=alpha_post, b=beta_post)

    plt.figure(figsize=(8, 4))
    plt.plot(x_grid, q_pdf, '-', label='Learned q(θ|y)')
    plt.plot(x_grid, true_pdf, '--', label='True Beta posterior')
    plt.xlabel('θ')
    plt.ylabel('Density')
    plt.title('Flow Approximation to Beta-Binomial Posterior')
    plt.legend()
    plt.tight_layout()
    plt.show()
```

```
# -------- Main Program --------
if __name__ == "__main__":

    all_y_obs = torch.tensor([7., 3., 4., 6., 2., 8., 5., 1., 9., 10.])  # p
    n_trials = 11
    alpha0, beta0 = 2.0, 5.0

    x = np.linspace(0.01, 0.99, 500)

    for N in [3]:
        print(f"\n--- Training with N = {N} observations ---")

        y_obs = all_y_obs[:N]  # select first N elements
        sum_y = y_obs.sum()
        alpha_post = alpha0 + sum_y
        beta_post = beta0 + N * n_trials - sum_y

        flow = AffineFlowLogit(obs_dim=N)
        train_flow(flow, y_obs, alpha0, beta0, n_trials)
        plot_density(flow, y_obs, x_grid=x, alpha_post=alpha_post.item(), be
```

```
--- Training with N = 3 observations ---
Training Flow: 100%|██████████| 1000/1000 [00:01<00:00, 941.93it/s]
```





Highlights

1. The results shows that we are fitting the true Beta posterior well.
2. We use n_trials = 10, and the number of experiments is 10, indeed , we will find that for N>=3, the fitting is good enough.
3. Here the result is not sensitive to the architecture of our NN, since the effect is quite similar for lr = 1e-2 or lr = 1e-3, and the epoch converges for epoch >200

Gamma as Posterior Example

We now try the case for Gamma-Poisson Example

Prior is Gamma(α,β) , and we obeserve $y_1, y_2 ..., y_n$ for each pair of theta

- Prior : $\theta \sim Gamma(\alpha_0, \beta_0)$
- Likelihood: $y_i \sim Poisson(\theta)$, i = 1,...,N

By conjugacy, the posterior will also be a Gamma distribution , and we are using a Normalising flow from standard normal distribution to this posterior

$$\theta \mid \mathbf{y} \sim \mathrm{Gamma}\left(\alpha_0 + \sum_i y_i,\ \beta_0 + N\right)$$

Define the Structure of Flow

We model the flow by transforming the latent variable (z) via an affine map in log-space:

$$\log \theta = a(\mathbf{y})\, z + b(\mathbf{y}),$$

which implies

$$\theta = \exp\bigl(a(\mathbf{y})\, z + b(\mathbf{y})\bigr) \;\in\; (0, \infty).$$

Change of Variables

We use the standard change-of-variables formula for the density:

$$q(\theta \mid y) = q(z) \left|\tfrac{d\theta}{dz}\right|^{-1}.$$

Taking logs gives

$$\log q(\theta \mid y) = \log q(z) - \log\left|\frac{d\theta}{dz}\right|.$$

Since

$$\theta = e^{az+b}, \quad \frac{d\theta}{dz} = a\, e^{az+b} = a\, \theta,$$

we obtain

$$\log q(\theta \mid y) = \log q(z) - \log|a| - \log|\theta|.$$

In code:

```
log_q = log_qz - torch.log(scale) - torch.log(theta)
```

ELBO Objective

Our target is to minimize the value of KL, ie, minimising the loss:

$$\mathcal{L}(\phi) = \mathbb{E}_{q_\phi(\theta|\mathbf{y})}\left[\log p(\theta) + \log p(\mathbf{y} \mid \theta) - \log q_\phi(\theta \mid \mathbf{y})\right]$$

- where we can compute $log(p(\theta))$ via Gamma;
- compute $logp(y|\theta)$ via Poisson
- compute $q(\theta|y)$ via change of variable

In [14]:
```
import torch
import torch.nn as nn
import torch.optim as optim
import matplotlib.pyplot as plt
from scipy.stats import gamma as gamma_dist
import numpy as np
from tqdm import trange
torch.manual_seed(0)
# -------- Base class for Flow --------
class BaseFlow(nn.Module):
    def __init__(self):
        super().__init__()
    def sample(self, batch_size, y_obs):
        """
        Sample θ from q(θ|y_obs)
```

```
        Returns:
            theta: shape (batch_size,)
            log_q: shape (batch_size,)
        """
        raise NotImplementedError
    def eval_log_prob(self, x_grid, y_obs):
        """
        Evaluate the approximate posterior density q(θ|y_obs) on a grid
        """
        raise NotImplementedError
```

In [15]:

```
# --------- Affine Exp Flow ---------
class AffineFlowExp(BaseFlow):
    def __init__(self, obs_dim):
        super().__init__()
        self.linear = nn.Linear(obs_dim, 2)

    def _get_params(self, y_obs):
        params = self.linear(y_obs.unsqueeze(0))  # shape (1, 2)
        log_scale = params[0, 0]
        shift     = params[0, 1]
        scale     = torch.exp(log_scale)
        return scale, shift

    def sample(self, batch_size, y_obs):
        z = torch.randn(batch_size)
        scale, shift = self._get_params(y_obs)
        log_theta = (scale * z + shift).clamp(min=-10, max=10)
        theta = torch.exp(log_theta).clamp(min=1e-6, max=1e2)

        # log q(θ|y_obs)
        log_qz = torch.distributions.Normal(0, 1).log_prob(z)
        log_jacobian = torch.log(theta)
        log_q = log_qz - torch.log(scale) - log_jacobian
        return theta, log_q

    def eval_log_prob(self, x_grid, y_obs):
        scale, shift = self._get_params(y_obs)
        x_t = torch.tensor(x_grid)
        log_x = torch.log(x_t)
        z_x = (log_x - shift) / scale
        log_qz = torch.distributions.Normal(0, 1).log_prob(z_x)
        log_qx = log_qz - torch.log(scale) - torch.log(x_t)
        return log_qx.exp().detach().numpy()
```

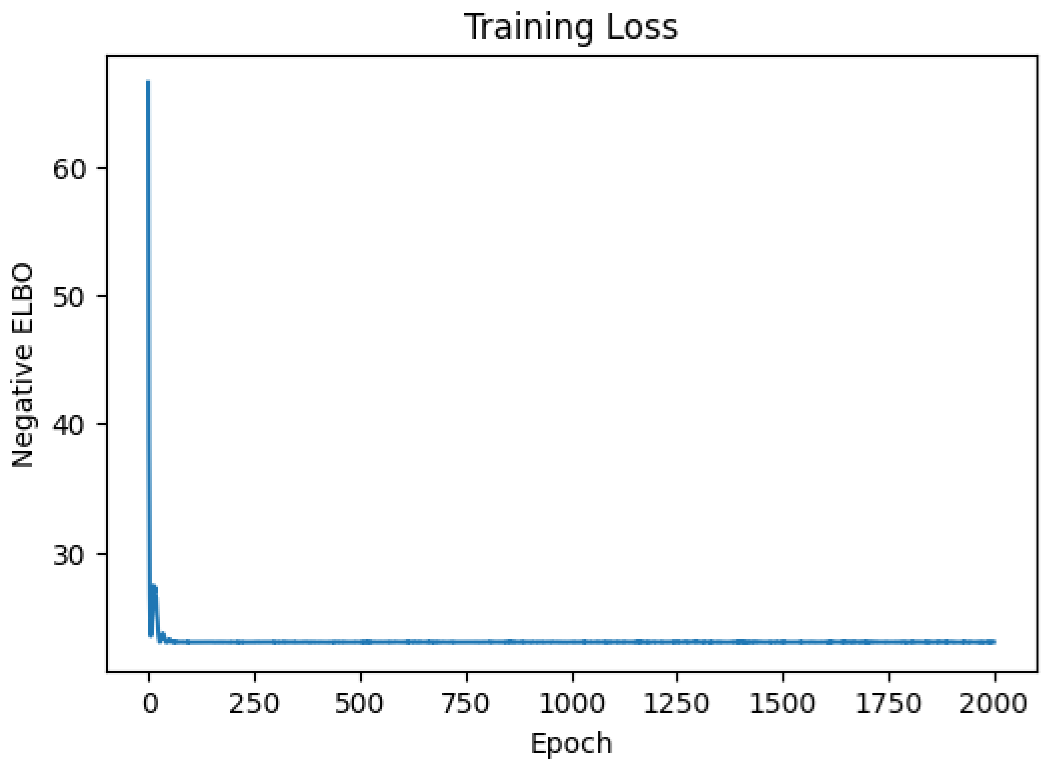
In [16]:

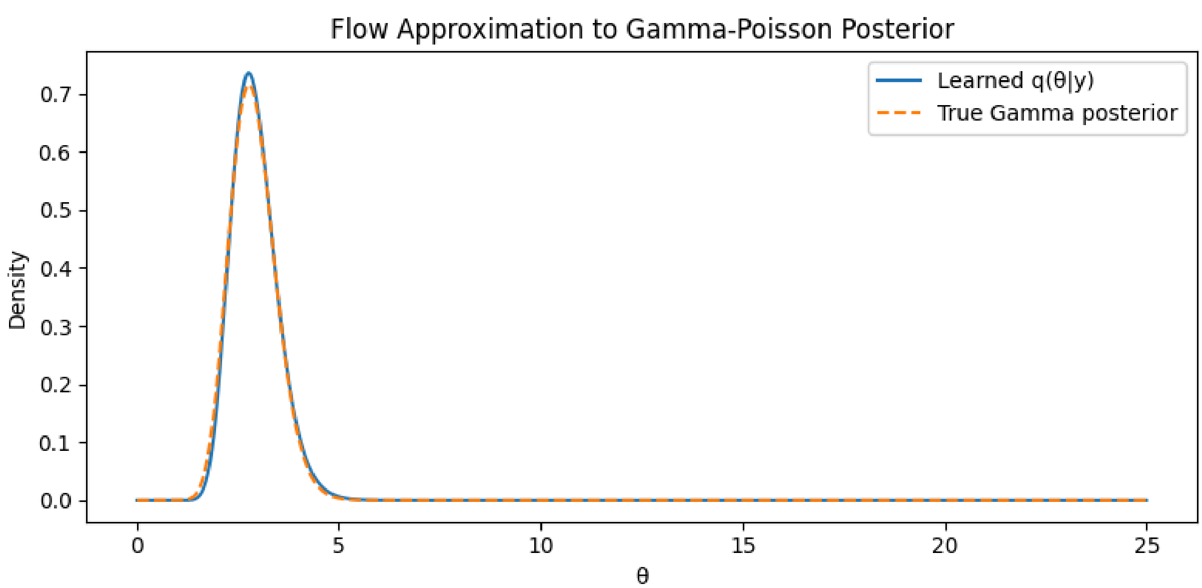
```
# --------- Training function ---------
def train_flow(flow, y_obs, alpha0, beta0, n_epochs=2000, n_samples=200, lr=
    optimizer = optim.Adam(flow.parameters(), lr=lr)
    N = y_obs.shape[0]
    losses = []
    for epoch in trange(n_epochs):
        optimizer.zero_grad()
        theta, log_q = flow.sample(n_samples, y_obs)

        # log p(θ)
```

```
        log_prior = torch.distributions.Gamma(alpha0, beta0).log_prob(theta)

        # log p(y | θ)
        theta_rep = theta.unsqueeze(1).expand(-1, N)
        y_rep = y_obs.unsqueeze(0).expand_as(theta_rep)
        log_lik = torch.distributions.Poisson(theta_rep).log_prob(y_rep).sum

        # ELBO
        elbo = (log_prior + log_lik - log_q).mean()
        loss = -elbo

        loss.backward()
        optimizer.step()
        losses.append(loss.item())
    plt.figure(figsize = (6,4))
    plt.plot(losses)
    plt.xlabel("Epoch")
    plt.ylabel("Negative ELBO")
    plt.title("Training Loss")
    plt.show()

# -------- Plotting function --------
def plot_density(flow, y_obs, x_grid, alpha_post, beta_post):
    q_pdf = flow.eval_log_prob(x_grid, y_obs)
    true_pdf = gamma_dist.pdf(x_grid, a=alpha_post, scale=1 / beta_post)

    plt.figure(figsize=(8, 4))
    plt.plot(x_grid, q_pdf, '-', label='Learned q(θ|y)')
    plt.plot(x_grid, true_pdf, '--', label='True Gamma posterior')
    plt.xlabel('θ')
    plt.ylabel('Density')
    plt.title('Flow Approximation to Gamma-Poisson Posterior')
    plt.legend()
    plt.tight_layout()
    plt.show()

# -------- Main Program --------
if __name__ == "__main__":
    # Observed data
    y_obs = torch.tensor([7., 4., 5., 8.])
    N = y_obs.shape[0]

    # Prior hyperparameters
    alpha0, beta0 = 2.0, 5.0

    # Posterior parameters for Gamma
    sum_y = y_obs.sum()
    alpha_post = alpha0 + sum_y
    beta_post  = beta0 + N

    # Grid for evaluation
    x = np.linspace(0.01, 25.0, 500)

    # Instantiate and train flow
    flow = AffineFlowExp(obs_dim=N)
    train_flow(flow, y_obs, alpha0, beta0)
```

```
    # Plot
    plot_density(flow, y_obs, x_grid=x, alpha_post=alpha_post, beta_post=bet
```

```
100%|██████████| 2000/2000 [00:00<00:00, 2428.87it/s]
```





Highlights

- With only 4 experiments, the fit is already very good.
- The model converges by around 200 epochs, so training for 2000 epochs is excessive.
- A learning rate of order $\leq 10^{-2}$ is sufficient.

- The model's performance is robust to the number of samples, provided there are at least 200.

Bivariate Normal as approximation to a Beta Posterior

Summary

Now we try the case for Beta Example based on standard bivariate normal distribution, because we want to estimate α and β at the same time.

We try to use the normalising flow that takes (z_1, z_2) as our input and our α and β as output. The structure of our flow is defined below:

$$z_{k+1} = A_k z_k + b_k$$

where the k represents the layer of our flow, because multiple flows is more expressive than single flow. Here we contains some clamping technique so the flow is not invertible, hence we only consider the forward procedure and different number layers would differ in the effects.

True Posterior

We observe data $y_1, y_2, \ldots, y_n \sim \text{Gamma}(\alpha, \beta)$, and our goal is to approximate the posterior distribution

$$p(\alpha, \beta \mid \mathbf{y})$$

using variational inference.

The prior is set as:

$$p(\alpha, \beta) = \text{Exp}(\lambda_\alpha) \cdot \text{Exp}(\lambda_\beta) = \lambda_\alpha e^{-\lambda_\alpha \alpha} \cdot \lambda_\beta e^{-\lambda_\beta \beta}$$

The unnormalized posterior is:

$$p(\alpha, \beta \mid \mathbf{y}) \propto \left[\prod_{i=1}^{n} \frac{\beta^\alpha}{\Gamma(\alpha)} y_i^{\alpha-1} e^{-\beta y_i} \right] \cdot e^{-\lambda_\alpha \alpha - \lambda_\beta \beta}$$

If we take a log on the posterior, we would obtain:

$$\log p(\alpha, \beta \mid y) = n\alpha \log \beta - n \log \Gamma(\alpha) + (\alpha - 1) \sum_{i=1}^{n} \log y_i - \beta \sum_{i=1}^{n} y_i - \lambda_\alpha \alpha - \lambda_\beta \beta$$

This can be calculated in python, and we are able to plot them, as shown below:

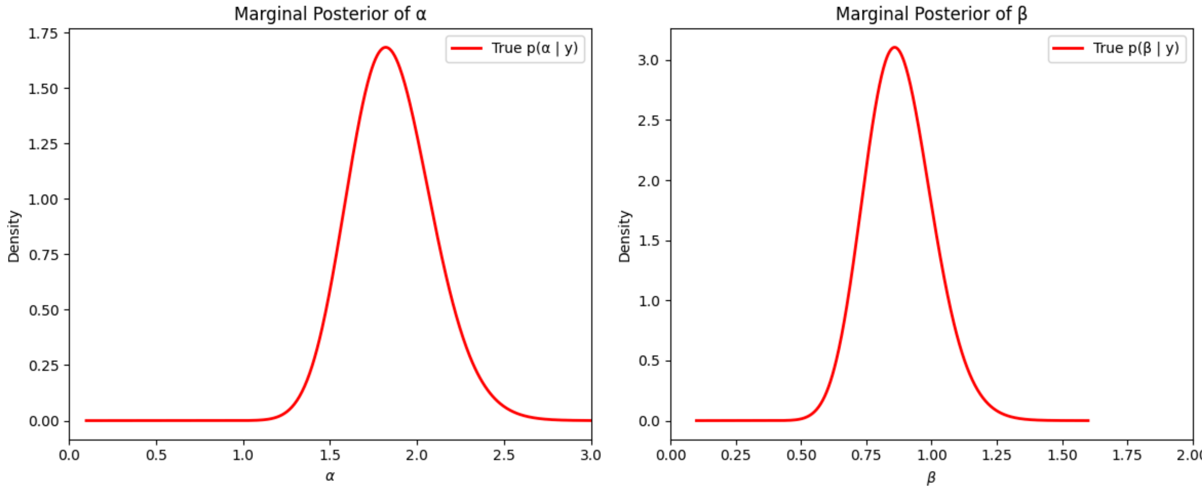
In [17]:
```
import os
import torch
```

```
import torch.nn as nn
import torch.optim as optim
import torch.nn.functional as F
from torch.distributions.normal import Normal
import scipy.stats as stats
from mpl_toolkits.mplot3d import Axes3D
import scipy.special as sp
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import scipy.special as sp


torch.manual_seed(123)
np.random.seed(123)

# %% 1. Data generation
true_alpha = 2.0    # Gamma shape parameter
true_beta  = 1.0    # Gamma rate parameter
num_obs    = 100    # Number of observations

# Generate observations y_i ~ Gamma(alpha, beta)
y_np = np.random.gamma(shape=true_alpha, scale=1.0 / true_beta, size=num_obs
y_tensor = torch.tensor(y_np, dtype=torch.float32)

# Save the data
np.savetxt("y_train_gamma.txt", y_np)  # save the data
# print("trainning set is y_train_gamma.txt")
```

In [18]:
```
# Load the dataset
# Allow non-duplicate loading of the KMP (Intel MKL) library
os.environ["KMP_DUPLICATE_LIB_OK"] = "TRUE"
# Reading the training data from local
y_np = np.loadtxt("y_train_gamma.txt")
y_tensor = torch.tensor(y_np, dtype=torch.float32)
num_obs = len(y_tensor)
# Sufficient statistics (used as input to the flow)
sum_log_y = torch.sum(torch.log(y_tensor)).item()
sum_y     = torch.sum(y_tensor).item()
mean_log_y = sum_log_y / num_obs
mean_y     = sum_y / num_obs
summary_stats = torch.tensor([mean_log_y, mean_y], dtype=torch.float32)

# Prior hyperparameters: Exponential(λ)
lambda_alpha = 1.0
lambda_beta  = 1.0
```

In [19]:
```
# Grids over alpha and beta
alpha_grid = np.linspace(0.1, 3.0, 600)     # horizontal axis (shape)
beta_grid  = np.linspace(0.1, 1.6, 600)     # vertical axis (rate)
AlphaGrid, BetaGrid = np.meshgrid(alpha_grid, beta_grid)

# Compute the unnormalized log posterior: log p(alpha, beta | y)
log_posterior_density = (
    num_obs * AlphaGrid * np.log(BetaGrid)
```

```
    - num_obs * sp.gammaln(AlphaGrid)
    + (AlphaGrid - 1) * sum_log_y
    - BetaGrid * sum_y
    - lambda_alpha * AlphaGrid
    - lambda_beta  * BetaGrid
)

# Step 1: Normalize the posterior (numerical stability)
log_posterior_density -= np.max(log_posterior_density)
posterior_density_true = np.exp(log_posterior_density)

d_alpha = alpha_grid[1] - alpha_grid[0]
d_beta  = beta_grid[1] - beta_grid[0]
posterior_density_true /= np.sum(posterior_density_true) * d_alpha * d_beta

# Step 2: Compute marginal densities
posterior_alpha_true = np.sum(posterior_density_true, axis=0) * d_beta  # p(
posterior_beta_true  = np.sum(posterior_density_true, axis=1) * d_alpha  # p

# Step 3: Plot estimated vs. true marginals
plt.figure(figsize=(12, 5))

# α marginal
plt.subplot(1, 2, 1)

plt.plot(alpha_grid, posterior_alpha_true, 'r-', linewidth=2, label='True p(
plt.xlabel(r'$\alpha$')
plt.ylabel('Density')
plt.title('Marginal Posterior of α')
plt.xlim(0, 3)
plt.legend()

# β marginal
plt.subplot(1, 2, 2)

plt.plot(beta_grid, posterior_beta_true, 'r-', linewidth=2, label='True p(β
plt.xlabel(r'$\beta$')
plt.ylabel('Density')
plt.title('Marginal Posterior of β')
plt.xlim(0, 2)
plt.legend()

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



These two figures give us the marginal posterior of α and β, and now we are using normalising flow to estimate the posterior.

Our Flow

The input is a tensor of shape `(batch_size, 2)`, sampled from the base distribution (typically `z ~ N(0, I)`). `summary` is laceholder argument (currently unused, but reserved for future conditional flows if needed).

This flow model applies `K` affine transformations to the input `z`, where each affine transformation is defined by a symmetric 2×2 matrix:

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{bmatrix}, \quad b \in \mathbb{R}^2$$

The update rule is:

$$z_{k+1} = A_k z_k + b_k$$

At each step, the log-determinant of the Jacobian (`log|det A_k|`) is accumulated to compute the total volume change introduced by the flow.

In [20]:
```
class StructuredComposedLinearFlow2D(nn.Module):
    """
    Composition of K structured linear affine flows:
    Each A_k is a 2x2 matrix with symmetry A[0,1] == A[1,0]
    A = [[a11, a12],
         [a12, a22]]
    """
    def __init__(self, num_flows=3):
        super().__init__()
        self.num_flows = num_flows
        self.a11s = nn.ParameterList() # The a11 in every flow
        self.a12s = nn.ParameterList() # The a12 in every flow
        self.a22s = nn.ParameterList() # The a22 in every flow
```

```
        self.bs   = nn.ParameterList() # The b in every flow

        for _ in range(num_flows):
            self.a11s.append(nn.Parameter(torch.tensor(1.0 + 0.01 * torch.ra
            self.a12s.append(nn.Parameter(torch.tensor(0.01 * torch.randn(()
            self.a22s.append(nn.Parameter(torch.tensor(1.0 + 0.01 * torch.ra
            self.bs.append(nn.Parameter(torch.zeros(2)))

    def forward(self, summary, z):
        z_k = z # Our initial z (from the base)
        log_det_total = 0.0 # Used later of change of variable

        for a11, a12, a22, b in zip(self.a11s, self.a12s, self.a22s, self.bs
            A = torch.stack([
                torch.stack([a11, a12]),
                torch.stack([a12, a22])
            ])
            z_k = z_k @ A.t() + b
            _, log_det_A = torch.slogdet(A)
            log_det_total += log_det_A

        alpha_q = torch.exp(z_k[:, 0])
        beta_q  = torch.exp(z_k[:, 1])

        log_p0 = Normal(0, 1).log_prob(z).sum(dim=1)
        log_det_exp = z_k.sum(dim=1)
        log_q = log_p0 - log_det_total - log_det_exp

        return alpha_q, beta_q, log_q
```

Training Process

Still, our target is to maximize the ELBO, and our loss is -ELBO:

$$\mathcal{L}(\phi) = \mathbb{E}_{q_\phi(\alpha,\beta|\mathbf{y})}\left[\log p(\alpha,\beta) + \log p(\mathbf{y} \mid \alpha,\beta) - \log q_\phi(\alpha,\beta \mid \mathbf{y})\right]$$

where

- Prior:

$$\log p(\alpha,\beta) = -\lambda_\alpha \alpha - \lambda_\beta \beta + \text{const}$$

- Log-Likelihood :

$$\log p(\alpha,\beta \mid y) = n\alpha \log\beta - n\log\Gamma(\alpha) + (\alpha-1)\sum_{i=1}^{n}\log y_i - \beta\sum_{i=1}^{n} y_i - \lambda_\alpha \alpha - \lambda_\beta$$

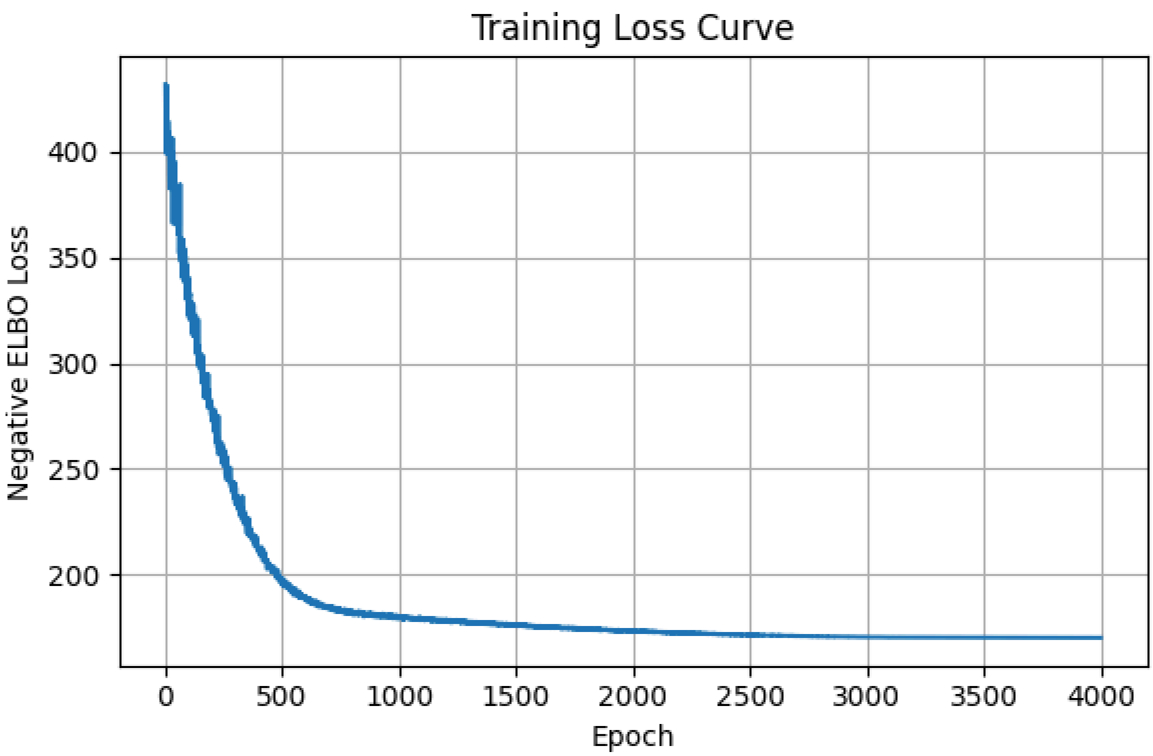
- Log_q:

$$\log q(\alpha,\beta) = \log p_0(\mathbf{z}) - \log|\det A| - \log\alpha - \log\beta$$

We set the number of flows to be 1 , with learning rate of 1e-3, we choose epoches of 4000, and sampling 2000.

In [21]:
```
flow_model = StructuredComposedLinearFlow2D(num_flows=1) # We have chosen ou

optimizer = optim.Adam(flow_model.parameters(), lr=1e-3)
base_dist = Normal(torch.zeros(2), torch.ones(2))

# %% 4. ELBO training
num_epochs = 4000
MC_samples = 2000

losses = []
for epoch in range(1, num_epochs + 1):
    z_sample = base_dist.sample((MC_samples,))
    alpha_q, beta_q, log_q = flow_model(summary_stats, z_sample)

    log_prior = -lambda_alpha * alpha_q - lambda_beta * beta_q
    log_likelihood = (
        num_obs * alpha_q * torch.log(beta_q.clamp(min=1e-8))
        - num_obs * torch.lgamma(alpha_q)
        + (alpha_q - 1) * sum_log_y
        - beta_q * sum_y
    )

    elbo = torch.mean(log_prior + log_likelihood - log_q)
    loss = -elbo

    optimizer.zero_grad()
    loss.backward()
    optimizer.step()

    if epoch % 500 == 0:
        print(f"Epoch {epoch:3d} | Loss = {loss.item():.4f}")
    losses.append(loss.item())

plt.figure(figsize=(6, 4))
plt.plot(losses)
plt.xlabel("Epoch")
plt.ylabel("Negative ELBO Loss")
plt.title("Training Loss Curve")
plt.grid(True)
plt.tight_layout()
plt.show()
```

```
/var/folders/bt/qcg_frss46xfvvsc6gdw2gd80000gn/T/ipykernel_75154/2570464328.
py:17: UserWarning: To copy construct from a tensor, it is recommended to us
e sourceTensor.clone().detach() or sourceTensor.clone().detach().requires_gr
ad_(True), rather than torch.tensor(sourceTensor).
  self.a11s.append(nn.Parameter(torch.tensor(1.0 + 0.01 * torch.randn(()))))
/var/folders/bt/qcg_frss46xfvvsc6gdw2gd80000gn/T/ipykernel_75154/2570464328.
py:18: UserWarning: To copy construct from a tensor, it is recommended to us
e sourceTensor.clone().detach() or sourceTensor.clone().detach().requires_gr
ad_(True), rather than torch.tensor(sourceTensor).
  self.a12s.append(nn.Parameter(torch.tensor(0.01 * torch.randn(()))))
/var/folders/bt/qcg_frss46xfvvsc6gdw2gd80000gn/T/ipykernel_75154/2570464328.
py:19: UserWarning: To copy construct from a tensor, it is recommended to us
e sourceTensor.clone().detach() or sourceTensor.clone().detach().requires_gr
ad_(True), rather than torch.tensor(sourceTensor).
  self.a22s.append(nn.Parameter(torch.tensor(1.0 + 0.01 * torch.randn(()))))
Epoch 500 | Loss = 196.9026
Epoch 1000 | Loss = 179.0935
Epoch 1500 | Loss = 175.6346
Epoch 2000 | Loss = 172.9167
Epoch 2500 | Loss = 171.3498
Epoch 3000 | Loss = 170.3006
Epoch 3500 | Loss = 169.9806
Epoch 4000 | Loss = 169.9396
```



Insight on Number of Flows

In theory, a sequence of purely affine flows can be collapsed into one:

$$f_2(f_1(z)) = A_2\big(A_1 z + b_1\big) + b_2 = (A_2 A_1)\, z + (A_2 b_1 + b_2).$$

However, because we apply the non-linear clamp

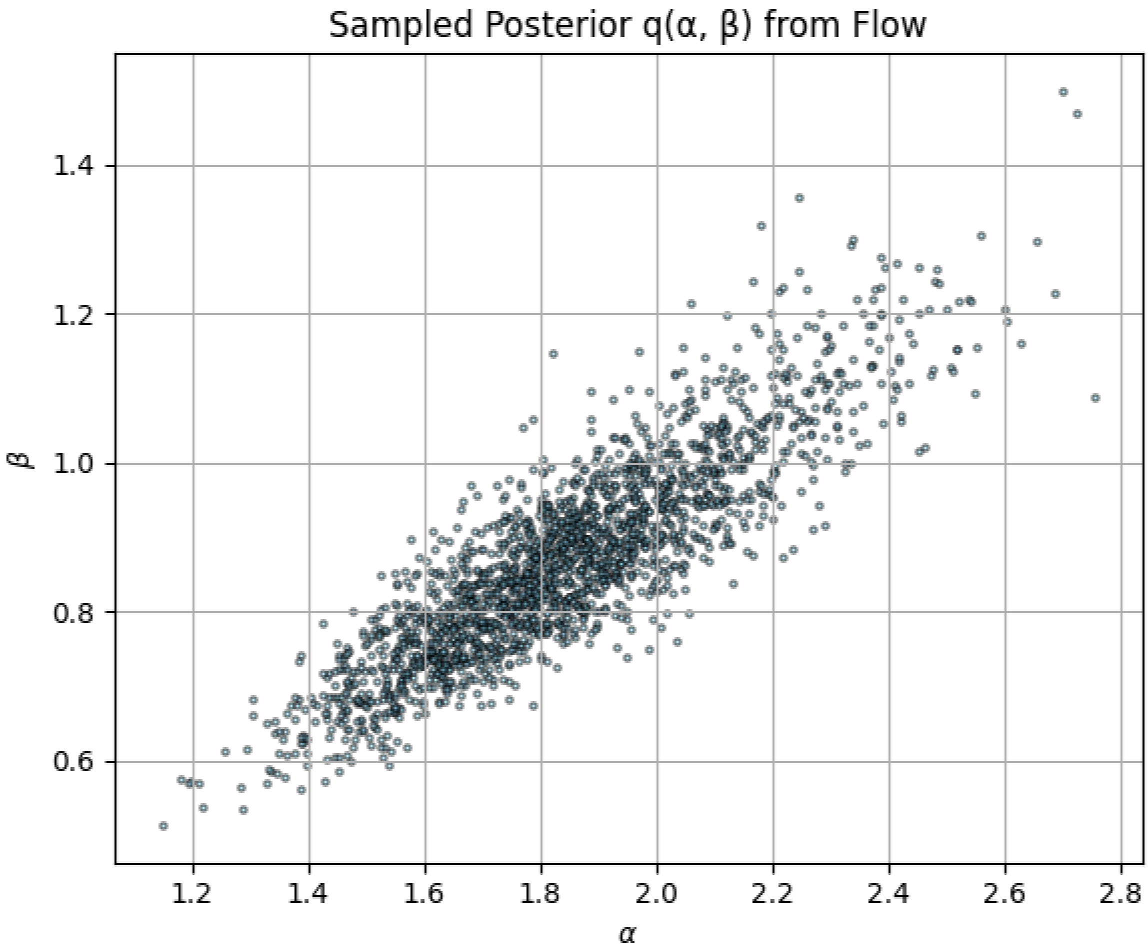
```
beta_q = beta_q.clamp(min=1e-8)
```

This is no longer the case. Stacking $K > 1$ flows does increase the model's capacity, but in our Beta-flow example the gains beyond $K = 1$ are marginal.

Practical choice: A single flow ($K = 1$) provides sufficient flexibility for this task, with minimal added complexity.

Thus, we proceed with flow 1 for our experiments.

In [22]:
```
import torch
import matplotlib.pyplot as plt
from torch.distributions import Normal

# Step 1: Sample from base distribution
base_dist = Normal(torch.zeros(2), torch.ones(2))
z_sample = base_dist.sample((2000,))  # Sample 3000 points

# Step 2: Pass through the trained flow model

dummy_summary = None
alpha_q, beta_q, log_q = flow_model(dummy_summary, z_sample)

# Step 3: Detach and convert to NumPy for plotting
alpha_np = alpha_q.detach().cpu().numpy()
beta_np  = beta_q.detach().cpu().numpy()

# Step 4: Plot scatter plot ("cloud")
plt.figure(figsize=(6, 5))
plt.scatter(alpha_np, beta_np, s=5, alpha=0.5, c='skyblue', edgecolor='k')
plt.xlabel(r'$\alpha$')
plt.ylabel(r'$\beta$')
plt.title('Sampled Posterior q(α, β) from Flow')
plt.grid(True)
plt.tight_layout()
plt.show()
```



Plotting the Estimated Posterior

1. Sample 2000 latent vectors

$$z^{(i)} \sim \mathcal{N}\big(0,\, I\big), \quad i = 1, \ldots, 2000.$$

2. Transform each via the trained flow to obtain Beta parameters:

$$(\alpha^{(i)},\, \beta^{(i)}) = f_\phi\big(z^{(i)}\big).$$

3. Draw posterior samples

$$\theta^{(i)} \sim \mathrm{Beta}\big(\alpha^{(i)},\, \beta^{(i)}\big).$$

4. Plot the histogram of $\{\theta^{(i)}\}$ and overlay the true posterior density

$$p(\theta \mid y_{\mathrm{obs}}) = \mathrm{Beta}\big(\alpha + y_{\mathrm{obs}},\, \beta + n - y_{\mathrm{obs}}\big).$$

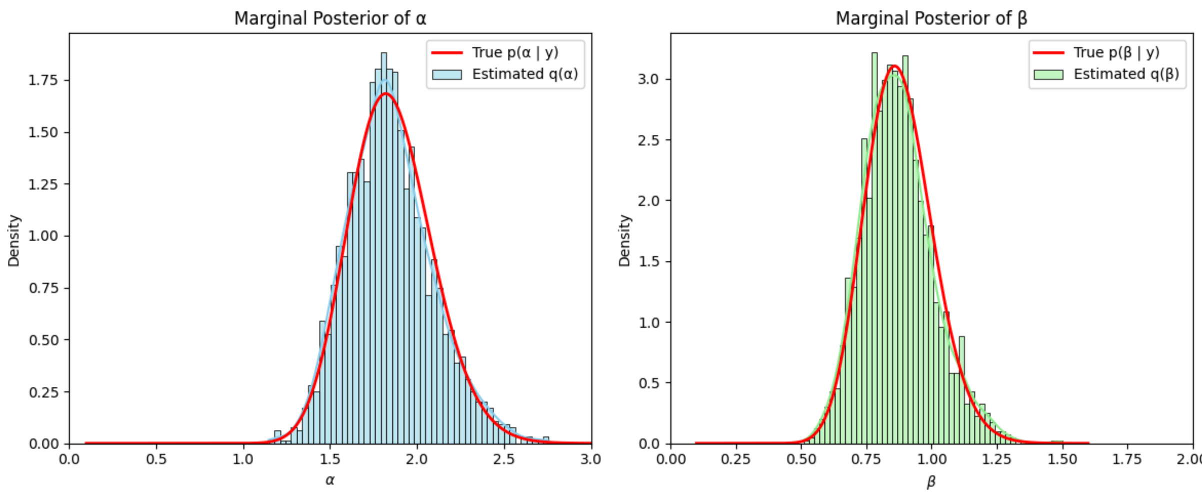
This visualization confirms that the flow-based approximation closely matches the true posterior.

In [31]:
```
# Indeed ,since it is linear tranformation, we can still calculate the inver
# A and b ,  so in theory we can do the inverse, now we define the inverse p
```

```
def evaluate_q(alpha_beta):  # input shape: [N, 2]
    z = alpha_beta
    for A, b in reversed(flow_layers):
        z = (z - b) @ torch.inverse(A).T
    log_p0 = Normal(0, 1).log_prob(z).sum(dim=1)  # log p(z)
    log_det = sum([torch.slogdet(A)[1] for A in flow_layers])  # constant
    log_q = log_p0 - log_det - alpha_beta.sum(dim=1)  # subtract Jacobian +
    return torch.exp(log_q)
```

In [32]:
```
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import scipy.special as sp

# Grids over alpha and beta
alpha_grid = np.linspace(0.1, 3.0, 600)     # horizontal axis (shape)
beta_grid  = np.linspace(0.1, 1.6, 600)     # vertical axis (rate)
AlphaGrid, BetaGrid = np.meshgrid(alpha_grid, beta_grid)

# Compute the unnormalized log posterior: log p(alpha, beta | y)
log_posterior_density = (
    num_obs * AlphaGrid * np.log(BetaGrid)
    - num_obs * sp.gammaln(AlphaGrid)
    + (AlphaGrid - 1) * sum_log_y
    - BetaGrid * sum_y
    - lambda_alpha * AlphaGrid
    - lambda_beta  * BetaGrid
)

# Step 1: Normalize the posterior (numerical stability)
log_posterior_density -= np.max(log_posterior_density)
posterior_density_true = np.exp(log_posterior_density)

d_alpha = alpha_grid[1] - alpha_grid[0]
d_beta  = beta_grid[1] - beta_grid[0]
posterior_density_true /= np.sum(posterior_density_true) * d_alpha * d_beta

# Step 2: Compute marginal densities
posterior_alpha_true = np.sum(posterior_density_true, axis=0) * d_beta  # p(
posterior_beta_true  = np.sum(posterior_density_true, axis=1) * d_alpha  # p

# Step 3: Plot estimated vs. true marginals
plt.figure(figsize=(12, 5))

# α marginal
plt.subplot(1, 2, 1)
sns.histplot(alpha_np, bins=50, stat='density', kde=True, color='skyblue', l
plt.plot(alpha_grid, posterior_alpha_true, 'r-', linewidth=2, label='True p(
plt.xlabel(r'$\alpha$')
plt.ylabel('Density')
plt.title('Marginal Posterior of α')
plt.xlim(0, 3)
plt.legend()

# β marginal
plt.subplot(1, 2, 2)
```

```
sns.histplot(beta_np, bins=50, stat='density', kde=True, color='lightgreen',
plt.plot(beta_grid, posterior_beta_true, 'r-', linewidth=2, label='True p(β
plt.xlabel(r'$\beta$')
plt.ylabel('Density')
plt.title('Marginal Posterior of β')
plt.xlim(0, 2)
plt.legend()

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



Highlights

- The fit is very good.
- Performance is robust to the number of flows; a single flow provides sufficient flexibility.
- The model converges by around 4000 epochs.
- A learning rate of 10^{-2} yields optimal results; similar performance holds for $\mathrm{lr} \leq 10^{-2}$.