Statistics for Experimental Physics

Part II: Bayesian Statistics

Assessed Problem Sheet 4

Due: 11 December 2024

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Based on the material originally designed by Alan Heavens

Hand in by 5 pm Thursday 11th December.

Please submit a project-like report (PDF) with the results, and a copy of your code included. There are no page limits.

1. Cosmology with Supernovae Ia

In this exercise, you will write **your own HMC code** to infer cosmological parameters from supernova Ia data. Do not use a package for the main HMC implementation, but you may use packages (e.g. corner.py) to display results.

Objectives:

1. Implement the cosmological distance-redshift relation for a flat universe
2. Build a Hamiltonian Monte Carlo sampler from scratch
3. Infer Ω_m (matter density) and h (Hubble constant) from real supernova data (Pantheon+ dataset: 1701 supernovae)
4. Assess convergence using trace plots, autocorrelation, and effective sample size
5. Explore how HMC parameters affect sampling efficiency

The Big Picture: Type Ia supernovae are "standard candles" with known intrinsic brightness. By measuring their apparent brightness at different redshifts, we can map the distance-redshift relation, which depends on the Universe's composition (Ω_m, Ω_v, h). This same technique led to the 1998 Nobel Prize discovery that the Universe's expansion is accelerating, revealing the existence of dark energy.

1.1. Background and Theory

Type Ia Supernovae: Standard Candles for Cosmology

Type Ia supernovae are thermonuclear explosions of white dwarfs that reach the Chandrasekhar limit (~1.4 solar masses), making them excellent **standard candles**:

- Nearly uniform peak luminosity ($L \approx 10^{43}$ erg/s) after empirical corrections
- Visible to cosmological distances (billions of light-years)
- Led to the 1998 Nobel Prize discovery of accelerating cosmic expansion (Perlmutter, Schmidt, Riess)

Cosmological Framework

The Universe is expanding, causing **cosmological redshift**:

$$z \equiv \frac{\lambda_{\text{observed}} - \lambda_{\text{emitted}}}{\lambda_{\text{emitted}}} = \frac{a(t_{\text{now}})}{a(t_{\text{emission}})} - 1$$

where $a(t)$ is the scale factor ($a = 1$ today).

Our goal is to measure the expansion rate and composition of the universe by observing supernovae at different redshifts. Because supernovae are standard candles with known intrinsic brightness, measuring their apparent brightness (magnitude) tells us their distance. By mapping how distance varies with redshift for many supernovae, we can reconstruct the expansion history, which is governed by the cosmological parameters Ω_m and h. Different values of these parameters produce different distance-redshift curves—this is what allows us to infer cosmology from supernova observations.

The expansion is governed by the **Friedmann equation**:

$$H(z)^2 = H_0^2 \left[\Omega_m (1+z)^3 + \Omega_k (1+z)^2 + \Omega_v\right]$$

Parameters:

- $H_0 = 100h$ km/s/Mpc: Hubble constant ($h \approx 0.7$, typical range 0.6-0.8)
- $\Omega_m \approx 0.3$: matter density parameter (typical range 0.2-0.4)
- $\Omega_v \approx 0.7$: dark energy density parameter
- $\Omega_k = 1 - \Omega_m - \Omega_v$: curvature parameter

We assume a **flat universe** ($\Omega_m + \Omega_v = 1$, $\Omega_k = 0$), well-supported by CMB observations.

Distance Measurements

The flux from a supernova of luminosity L at **luminosity distance** D_L is:

$$f = \frac{L}{4\pi D_L^2}$$

For a flat universe, D_L is given by:

$$D_L(z) = 3000 h^{-1} (1+z) \int_0^z \frac{dz'}{\sqrt{\Omega_m (1+z')^3 + 1 - \Omega_m}} \text{ Mpc}$$

Since HMC requires millions of likelihood evaluations, we use the **Pen (1999) analytical approximation** (accurate to <0.4%):

$$D_L(z;\Omega_m,h) = \frac{c}{H_0}(1+z)\left[\eta(1,\Omega_m) - \eta\left(\frac{1}{1+z},\Omega_m\right)\right]$$

where $c = 299792.458$ km/s and:

$$\eta(a,\Omega_m) = 2\sqrt{s^3+1}\left[\frac{1}{a^4} - 0.1540\frac{s}{a^3} + 0.4304\frac{s^2}{a^2} + 0.19097\frac{s^3}{a} + 0.066941 s^4\right]^{-1/8}$$

with $s^3 = (1-\Omega_m)/\Omega_m$ and $a = 1/(1+z)$ (valid for $0.2 \leq \Omega_m \leq 1$).

Astronomers measure brightness using **magnitudes** ($m = -2.5\log_{10} f + \text{const}$). The **distance modulus** is:

$$\mu = m - M = 5\log_{10}\left(\frac{D_L}{\text{Mpc}}\right) + 25$$

Factoring out h using $D_L^* \equiv D_L(h=1)$:

$$\mu(z;\Omega_m,h) = 25 - 5\log_{10} h + 5\log_{10}\left(\frac{D_L^*}{\text{Mpc}}\right)$$

where h produces a vertical shift and Ω_m affects the curve shape.

1.2. Data

The data file (from the 'Pantheon+' sample - see https://arxiv.org/abs/2112.03863 for more detail) consists of data from 1701 supernovae, with a redshift and distance modulus μ for each supernova.

The file `Pantheon+SH0ES.dat` (from Teams or Blackboard) contains the data:

- `zHD` : redshift you should use
- `MU_SH0ES` : distance modulus

The covariance matrix C is provided in `Pantheon+SH0ES_STAT+SYS.cov.txt` (from Teams or Blackboard). It is a square symmetric matrix N x N. The file provided contains a vector (the first row is the size N) which you can just reshape to N x N.

The files can also be downloaded here:

- https://www.dropbox.com/scl/fi/n67of2kwtmabb2vahk36m/Pantheon-SH0ES.dat?rlkey=mw210zbna7b0pxs4ptj2gdivl&dl=0
- https://www.dropbox.com/scl/fi/ncafbjkwh5w83hehs6p0u/Pantheon-SH0ES_STAT-SYS.cov.txt.zip?rlkey=ruxgi74dkz1hcfehxdl4jfns9&dl=0

1.3. Exercise

Write your own HMC code to infer h and Ω_m from the supernova dataset, assuming the Universe is flat and the errors are Gaussian.

Requirements:

- Nearby supernovae have redshifts significantly altered by 'peculiar velocities', not associated with the general expansion of the Universe. **Discard supernovae with $z < 0.01$.**
- h and Ω_m are positive, and have values of the rough order of unity
- Assume uniform priors on the parameters (so you will sample from the likelihood)
- Explore visually (with trace plots) the chain, and compute and report the acceptance rate
- Choose a suitable burn-in and say why you chose it
- Compute the average value of the parameters under the posterior distribution, and their variances and covariance
- Compute and display the correlation function of the chain. Compute the acceptance rate and the effective number of samples, using the formula in the lectures. Explore how these changes as the parameters of the HMC are varied

My Report - Mihir Koka

Bayesian Inference of Cosmological Parameters from Supernova Ia Data

Student: Mihir Koka
Course: Statistics for Experimental Physics (Part II: Bayesian Statistics)
Date: December 2024

Quick Summary

This report implements a Hamiltonian Monte Carlo (HMC) sampler from scratch to infer cosmological parameters Ω_m (matter density) and h (reduced Hubble constant) from the Pantheon+ Type Ia supernova dataset. Key findings:

- Posterior mean: $\Omega_m = 0.329 \pm 0.017$, $h = 0.735 \pm 0.002$
- Effective sample size: $N_{\text{eff}} = 256$ (Ω_m), 382 (h)
- Acceptance rate: 90.9%

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1. Introduction

Type Ia supernovae are cosmological "standard candles" used to measure cosmic expansion. This project:

1. Implements the Pen (1999) distance-redshift approximation
2. Builds an HMC sampler without external MCMC packages
3. Diagnoses convergence via trace plots, autocorrelation, and ESS
4. Explores tuning parameter effects (ϵ, L)

Note: AI Declaration

AI was used in the following ways in this assignment:

- formatting my handwriting to LaTeX
- plotting functions (copilot tab complete)
- tables to output values, to format them nicely

In [2]:
```
# Import necessary libraries
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
import torch
torch.set_default_dtype(torch.float64)
from pathlib import Path

# Add your imports here
```

2. Data Preparation

Dataset: Pantheon+ (1701 SNe) filtered to $z \geq 0.01$ (removes peculiar velocity contamination)

In [3]:
```
# Load supernova data
# Filter z < 0.01
# Your code here

DATA_DIR = Path(".")
SN_FILE = DATA_DIR/"Pantheon+SH0ES.dat"
COV_FILE = DATA_DIR / "Pantheon+SH0ES_STAT+SYS.cov.txt"

df = pd.read_csv(SN_FILE, delim_whitespace=True)
expected_columns = {"zHD", "MU_SH0ES"}
print(set(df.columns).issuperset(expected_columns))

# Discard nearby SNe with z < 0.01, preserve original ordering
mask = df["zHD"].to_numpy() >= 0.01
idx = np.where(mask)[0]

df_f = df.loc[mask].reset_index(drop=True)
```

```
z_data = df_f["zHD"].to_numpy(dtype=np.float64)
mu_data = df_f["MU_SH0ES"].to_numpy(dtype=np.float64)

print(f"Loaded {len(df)} SNe; kept {len(z_data)} with z >= 0.01")
print(f"Data columns: {list(df.columns)}")
```

```
True
Loaded 1701 SNe; kept 1590 with z >= 0.01
Data columns: ['CID', 'IDSURVEY', 'zHD', 'zHDERR', 'zCMB', 'zCMBERR', 'zHEL', 'zHELE
RR', 'm_b_corr', 'm_b_corr_err_DIAG', 'MU_SH0ES', 'MU_SH0ES_ERR_DIAG', 'CEPH_DIST',
'IS_CALIBRATOR', 'USED_IN_SH0ES_HF', 'c', 'cERR', 'x1', 'x1ERR', 'mB', 'mBERR', 'x
0', 'x0ERR', 'COV_x1_c', 'COV_x1_x0', 'COV_c_x0', 'RA', 'DEC', 'HOST_RA', 'HOST_DE
C', 'HOST_ANGSEP', 'VPEC', 'VPECERR', 'MWEBV', 'HOST_LOGMASS', 'HOST_LOGMASS_ERR',
'PKMJD', 'PKMJDERR', 'NDOF', 'FITCHI2', 'FITPROB', 'm_b_corr_err_RAW', 'm_b_corr_err
_VPEC', 'biasCor_m_b', 'biasCorErr_m_b', 'biasCor_m_b_COVSCALE', 'biasCor_m_b_COVAD
D']
```

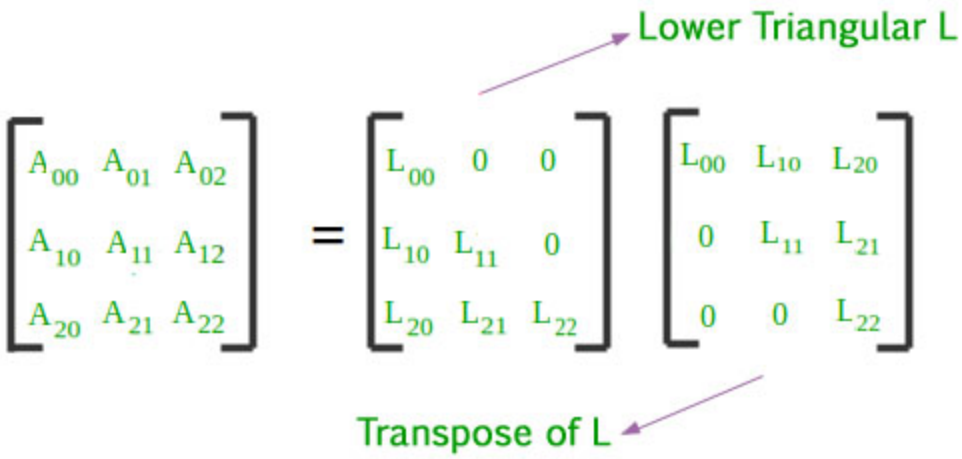
```
C:\Users\Mihir Koka\AppData\Local\Temp\ipykernel_25508\3155238785.py:9: FutureWarnin
g: The 'delim_whitespace' keyword in pd.read_csv is deprecated and will be removed i
n a future version. Use ``sep='\s+'`` instead
  df = pd.read_csv(SN_FILE, delim_whitespace=True)
```

Symmetrize: The file should store a symmetric matrix, but floating-point I/O can introduce tiny asymmetries. Forcing symmetry prevents numerical issues.

Jitter: Real covariance matrices can be nearly singular (almostzero eigenvalues) due to correlated systematic errors. Adding 1e-10 * mean ensures Cholesky doesn't fail. This is standard practice

Cholesky: We need to compute r^T C^-1 r millions of times. Direct inversion is:

- Slower ($O(N^3)$ time complexity per sample)
- Numerically unstable
  So we use a faster triangular solve, cholesky is needed to make our HMC efficient It gives us a lower trianglar matrix L s.t C = L L^T



In [4]:
```
# Load covariance matrix and extract corresponding subset after filtering
def load_covariance_vector_file(path: Path):
    """
    Load covariance from a file that stores N on the first line,
```

```
    followed by N*N values (vectorized). Returns C (N x N).
    """
    with open(path, "r") as f:
        first_line = f.readline().strip()
        N = int(first_line)
        flat = np.loadtxt(f, dtype=np.float64)

    assert flat.size == N * N, f"Expected {N*N} elements, got {flat.size}"
    C = flat.reshape(N, N)
    return C

C = load_covariance_vector_file(COV_FILE)

# Subset to match the filtered data indices
C_sub = C[np.ix_(idx, idx)].astype(np.float64)

# Symmetrize and add tiny jitter
C_sub = (C_sub + C_sub.T) / 2.0
jitter = 1e-10 * np.mean(np.diag(C_sub))
C_sub_j = C_sub + np.eye(C_sub.shape[0]) * jitter

# Cholesky decomposition
L = np.linalg.cholesky(C_sub_j)

print(f"Covariance original shape: {C.shape}, subset shape: {C_sub.shape}")

# Prepare torch tensors
z_t = torch.from_numpy(z_data)
mu_t = torch.from_numpy(mu_data)
C_chol_t = torch.from_numpy(L)
```

```
Covariance original shape: (1701, 1701), subset shape: (1590, 1590)
```

Implement the theoretical model (Pen 1999 formula)

3. Theoretical Model

Using the constants from the paper as seen here link to paper

Without further ado, the luminosity distance is given as

$$d_L = \frac{c}{H_0}(1+z)\left[\eta(1,\Omega_0) - \eta\left(\frac{1}{1+z},\Omega_0\right)\right],$$

$$\eta(a,\Omega_0) = 2\sqrt{s^3+1}\left[\frac{1}{a^4} - 0.1540\,\frac{s}{a^3} + 0.4304\,\frac{s^2}{a^2} + 0.19097\,\frac{s^3}{a} + 0.066941 s^4\right]^{-1/8},$$

$$s^3 = \frac{1-\Omega_0}{\Omega_0}. \qquad (1)$$

In [5]:

```python
def eta(a, Omega_m):
    """
    Helper function for Pen (1999) formula.

    Parameters:
    -----------
    a : float or array
        Scale factor (a = 1/(1+z))
    Omega_m : float
        Matter density parameter

    Returns:
    --------
    eta : float or array
    """
    s3 =(1.0 - Omega_m) / Omega_m
    s = s3**(1.0/3.0)

    #numerator
    term1 = 1.0 / (a**4)
    term2 = 0.1540 * s / (a**3)
    term3 = 0.4304 * (s**2) / (a**2)
    term4 = 0.19097 * (s**3) / a
    term5 = 0.066941 * (s**4)

    poly = term1 - term2 + term3 + term4 + term5

    eta_val = 2.0 * torch.sqrt(s3 + 1.0) * (poly ** (-1.0/8.0))
    return eta_val

def luminosity_distance_star(z, Omega_m):
    """
    Calculate D_L^* (luminosity distance with h=1 factored out) using Pen (1999).

    Parameters:
    -----------
    z : float or array
        Redshift
    Omega_m : float
        Matter density parameter

    Returns:
    --------
    D_L_star : float or array
        Luminosity distance in Mpc (with h=1)
    """
    c_km_s = 299792.458  # Speed of light in km/s

    # Compute eta at a=1 and a=1/(1+z)
    eta_1 = eta(torch.tensor(1.0, dtype=torch.float64), Omega_m)
    a_z = 1.0 / (1.0 + z)
    eta_z = eta(a_z, Omega_m)

    # D_L^* in Mpc
    D_L_star = (c_km_s / 100.0) * (1.0 + z) * (eta_1 - eta_z)
```

```
    return D_L_star

def distance_modulus(z, Omega_m, h):
    """
    Calculate theoretical distance modulus.

    Parameters:
    -----------
    z : float or array
        Redshift
    Omega_m : float
        Matter density parameter
    h : float
        Reduced Hubble constant

    Returns:
    --------
    mu : float or array
        Distance modulus
    """
    D_L_star = luminosity_distance_star(z, Omega_m)

    mu = 25.0 - 5.0 * torch.log10(h) + 5.0 * torch.log10(D_L_star)
    return mu


# === VALIDATION TEST ===
# Expected: Omega_m=0.3, h=0.7, z=0.5 → mu ≈ 42.3 mag (Pen 1999 approximation)
z_test = torch.tensor([0.5], dtype=torch.float64)
Omega_m_test = torch.tensor(0.3, dtype=torch.float64)
h_test = torch.tensor(0.7, dtype=torch.float64)

mu_test = distance_modulus(z_test, Omega_m_test, h_test)
print(f"Test: z={z_test.item():.1f}, Omega_m={Omega_m_test.item():.1f}, h={h_test.i
print(f"  → mu = {mu_test.item():.2f} mag (expect ~42.3)")

# Test on array of redshifts (should be monotonically increasing)
z_array = torch.tensor([0.1, 0.5, 1.0, 1.5], dtype=torch.float64)
mu_array = distance_modulus(z_array, Omega_m_test, h_test)
print(f"\nDistance moduli for z={z_array.numpy()}:")
for z_val, mu_val in zip(z_array, mu_array):
    print(f"  z={z_val:.1f} → μ={mu_val:.2f} mag")
```

```
Test: z=0.5, Omega_m=0.3, h=0.7
  → mu = 42.27 mag (expect ~42.3)

Distance moduli for z=[0.1 0.5 1.  1.5]:
  z=0.1 → μ=38.32 mag
  z=0.5 → μ=42.27 mag
  z=1.0 → μ=44.10 mag
  z=1.5 → μ=45.19 mag
```

Statistics seems to be within expectations and the magnitude is increasing smoothly.
Validation done.

Implement the likelihood and its gradient

4. HMC Implementation

In [6]:

```python
def log_likelihood(params, z_data, mu_data, C_chol):
    """
    Calculate log-likelihood for supernova data.

    Parameters:
    -----------
    params : torch.Tensor
        [Omega_m, h] (both must be positive)
    z_data : torch.Tensor
        Redshift data
    mu_data : torch.Tensor
        Observed distance modulus
    C_chol : torch.Tensor
        Cholesky factor L (lower triangular) where C = L L^T

    Returns:
    --------
    log_L : torch.Tensor (scalar)
        Log-likelihood value
    """
    Omega_m, h = params

    # Compute theoretical predictions
    mu_theory = distance_modulus(z_data, Omega_m, h)

    # Residuals
    r = mu_data - mu_theory

    # Solve L y = r (reshape r to column vector for solve_triangular)
    y = torch.linalg.solve_triangular(C_chol, r.unsqueeze(1), upper=False).squeeze(

    # chi^2 = r^T C^{-1} r = y^T y
    chi2 = torch.dot(y, y)

    # Log-likelihood (ignoring constant terms)
    log_L = -0.5 * chi2

    return log_L


def gradient_log_likelihood(params, z_data, mu_data, C_chol):
    """
    Calculate gradient using PyTorch autograd.

    Parameters:
    -----------
    params : torch.Tensor
        [Omega_m, h] with requires_grad=True
    z_data : torch.Tensor
        Redshift data
    mu_data : torch.Tensor
        Distance modulus data
```

```
    C_chol : torch.Tensor
        Cholesky factor

    Returns:
    --------
    grad : torch.Tensor
        Gradient [d(log L)/d(Omega_m), d(log L)/dh]
    """
    # Enable gradient tracking for autograd
    params_grad = params.clone().detach().requires_grad_(True)

    # Compute log-likelihood
    log_L = log_likelihood(params_grad, z_data, mu_data, C_chol)

    # Backpropagate to get gradients
    log_L.backward()

    return params_grad.grad.clone()


# === VALIDATION TEST ===
# Test likelihood at true cosmology (should be close to maximum)
params_test = torch.tensor([0.3, 0.7], dtype=torch.float64)
log_L_test = log_likelihood(params_test, z_t, mu_t, C_chol_t)
print(f"\nLog-likelihood at (Ωₘ=0.3, h=0.7): {log_L_test.item():.2f}")

# Test gradient (should be close to zero at maximum likelihood)
grad_test = gradient_log_likelihood(params_test, z_t, mu_t, C_chol_t)
print(f"Gradient at (Ωₘ=0.3, h=0.7): {grad_test.numpy()}")
print(f"Gradient magnitude: {torch.norm(grad_test).item():.2e}")
```

```
Log-likelihood at (Ωₘ=0.3, h=0.7): -1165.89
Gradient at (Ωₘ=0.3, h=0.7): [ 2525.49044828 25047.9376672 ]
Gradient magnitude: 2.52e+04
```

The log-likelihood indicates a resonable model -> data agreement. While the large magnitude shows that (Ω_m=0.3, h=0.7) is not at the max likelihood. The gradient is pointing toward better fit params. This validates that out gradient comp is working as expected and will guide the HMC towards the true posterior.

Implement HMC sampler

Implement the Hamiltonian Monte Carlo algorithm, including:

- Leapfrog integrator for Hamiltonian dynamics
- Metropolis acceptance step
- Main HMC loop

In [9]:

```
def leapfrog(q, p, epsilon, L, grad_log_prob, *args):
    """
    Leapfrog integrator for Hamiltonian dynamics.

    Parameters:
    -----------
```

```
    q : torch.Tensor
        Current position (parameters)
    p : torch.Tensor
        Current momentum
    epsilon : float
        Step size
    L : int
        Number of leapfrog steps
    grad_log_prob : function
        Function to calculate gradient of log probability
    *args : additional arguments
        Additional arguments to pass to grad_log_prob

    Returns:
    --------
    q_new : torch.Tensor
        New position
    p_new : torch.Tensor
        New momentum
    """
    q = q.clone()
    p = p.clone()

    # Half step for momentum at the beginning
    p = p + 0.5 * epsilon * grad_log_prob(q, *args)

    # Alternate full steps for position and momentum
    for i in range(L - 1):
        q = q + epsilon * p
        p = p + epsilon * grad_log_prob(q, *args)

    # Full step for position at the end
    q = q + epsilon * p

    # Half step for momentum at the end
    p = p + 0.5 * epsilon * grad_log_prob(q, *args)

    # Negate momentum for reversibility
    p = -p

    return q, p


def hmc_sampler(initial_params, n_samples, epsilon, L, log_prob, grad_log_prob, *ar
    """
    Hamiltonian Monte Carlo sampler.

    Parameters:
    -----------
    initial_params : torch.Tensor
        Initial parameter values [Omega_m, h]
    n_samples : int
        Number of samples to generate
    epsilon : float
        Step size for leapfrog integrator
    L : int
```

```
    Number of leapfrog steps per iteration
log_prob : function
    Log probability function
grad_log_prob : function
    Gradient of log probability
*args : additional arguments
    Additional arguments to pass to log_prob and grad_log_prob

Returns:
--------
samples : np.ndarray
    MCMC samples (n_samples x n_params)
acceptance_rate : float
    Fraction of proposals accepted
"""
n_params = len(initial_params)
samples = np.zeros((n_samples, n_params))
n_accepted = 0

# Initialize
q = initial_params.clone()

for i in range(n_samples):
    # Sample momentum from standard normal
    p = torch.randn(n_params, dtype=torch.float64)

    # Store current state
    q_current = q.clone()
    p_current = p.clone()

    # Compute current Hamiltonian
    current_log_prob = log_prob(q_current, *args)
    current_K = 0.5 * torch.dot(p_current, p_current)
    current_H = -current_log_prob + current_K

    # Leapfrog integration
    q_proposed, p_proposed = leapfrog(q_current, p_current, epsilon, L, grad_lo

    # Compute proposed Hamiltonian
    proposed_log_prob = log_prob(q_proposed, *args)
    proposed_K = 0.5 * torch.dot(p_proposed, p_proposed)
    proposed_H = -proposed_log_prob + proposed_K

    # Metropolis acceptance
    log_accept_ratio = current_H - proposed_H

    if torch.log(torch.rand(1, dtype=torch.float64)) < log_accept_ratio:
        q = q_proposed
        n_accepted += 1

    # Store sample
    samples[i] = q.numpy()

    # Progress indicator
    if (i + 1) % 100 == 0:
        print(f"Sample {i+1}/{n_samples}, acceptance rate: {n_accepted/(i+1):.2
```

```
    acceptance_rate = n_accepted / n_samples

    return samples, acceptance_rate


# === VALIDATION TEST ===
# Quick test with 10 samples
print("Testing HMC with 10 samples...")
initial_test = torch.tensor([0.3, 0.7], dtype=torch.float64)
samples_test, acc_test = hmc_sampler(
    initial_test,
    10,  # n_samples
    1e-4,  # epsilon
    20,  # L
    log_likelihood,  # log_prob
    gradient_log_likelihood,  # grad_log_prob
    z_t, mu_t, C_chol_t  # *args
)
print(f"\nTest completed. Acceptance rate: {acc_test:.2%}")
print(f"Sample mean: Ωₘ={samples_test[:, 0].mean():.3f}, h={samples_test[:, 1].mean

#report convergence, effecgive sample size, diagnostics in general
```

```
Testing HMC with 10 samples...

Test completed. Acceptance rate: 100.00%
Sample mean: Ωₘ=0.300, h=0.738
```

So with this small sample for sanity we got a 100% acceptance. This means our epsilon is taking tiny steps and thus everything is being accepted. But due to that it's exploring very slowly.

Run HMC sampler

In [41]:
```
# Set HMC parameters
initial_params = torch.tensor([0.3, 0.7], dtype=torch.float64)
n_samples = 10000  # sample size
epsilon = 2e-3    # step size
L = 50           # number of leapfrog steps

# Run HMC
print("Running full HMC chain...")
print(f"Configuration: N={n_samples}, ε={epsilon:.0e}, L={L}")
print("-" * 60)

samples, acceptance_rate = hmc_sampler(
    initial_params, n_samples, epsilon, L,
    log_likelihood, gradient_log_likelihood,
    z_t, mu_t, C_chol_t
)
print("\n" + "=" * 60)
print("SAMPLING COMPLETE")
print("=" * 60)
print(f"Final acceptance rate: {acceptance_rate:.1%}")
```

```
print(f"Total samples: {n_samples}")
print(f"Posterior mean: Ωₘ={samples[:, 0].mean():.4f}, h={samples[:, 1].mean():.4f}
print(f"Posterior std:  Ωₘ={samples[:, 0].std():.4f}, h={samples[:, 1].std():.4f}")
```

```
Running full HMC chain...
Configuration: N=10000, ε=2e-03, L=50
------------------------------------------------------------
Sample 100/10000, acceptance rate: 33.00%
Sample 200/10000, acceptance rate: 60.50%
Sample 300/10000, acceptance rate: 71.33%
Sample 400/10000, acceptance rate: 76.75%
Sample 500/10000, acceptance rate: 80.00%
Sample 600/10000, acceptance rate: 81.83%
Sample 700/10000, acceptance rate: 83.14%
Sample 800/10000, acceptance rate: 84.12%
Sample 900/10000, acceptance rate: 84.89%
Sample 1000/10000, acceptance rate: 85.50%
Sample 1100/10000, acceptance rate: 85.64%
Sample 1200/10000, acceptance rate: 86.67%
Sample 1300/10000, acceptance rate: 87.00%
Sample 1400/10000, acceptance rate: 87.29%
Sample 1500/10000, acceptance rate: 87.93%
Sample 1600/10000, acceptance rate: 88.62%
Sample 1700/10000, acceptance rate: 88.76%
Sample 1800/10000, acceptance rate: 89.00%
Sample 1900/10000, acceptance rate: 88.95%
Sample 2000/10000, acceptance rate: 89.30%
Sample 2100/10000, acceptance rate: 89.29%
Sample 2200/10000, acceptance rate: 89.50%
Sample 2300/10000, acceptance rate: 89.61%
Sample 2400/10000, acceptance rate: 89.83%
Sample 2500/10000, acceptance rate: 89.80%
Sample 2600/10000, acceptance rate: 89.88%
Sample 2700/10000, acceptance rate: 89.96%
Sample 2800/10000, acceptance rate: 89.86%
Sample 2900/10000, acceptance rate: 89.83%
Sample 3000/10000, acceptance rate: 89.93%
Sample 3100/10000, acceptance rate: 89.90%
Sample 3200/10000, acceptance rate: 89.91%
Sample 3300/10000, acceptance rate: 90.09%
Sample 3400/10000, acceptance rate: 90.15%
Sample 3500/10000, acceptance rate: 90.09%
Sample 3600/10000, acceptance rate: 90.06%
Sample 3700/10000, acceptance rate: 90.00%
Sample 3800/10000, acceptance rate: 89.92%
Sample 3900/10000, acceptance rate: 90.00%
Sample 4000/10000, acceptance rate: 90.15%
Sample 4100/10000, acceptance rate: 90.10%
Sample 4200/10000, acceptance rate: 90.24%
Sample 4300/10000, acceptance rate: 90.30%
Sample 4400/10000, acceptance rate: 90.36%
Sample 4500/10000, acceptance rate: 90.40%
Sample 4600/10000, acceptance rate: 90.41%
Sample 4700/10000, acceptance rate: 90.40%
Sample 4800/10000, acceptance rate: 90.33%
Sample 4900/10000, acceptance rate: 90.35%
Sample 5000/10000, acceptance rate: 90.38%
Sample 5100/10000, acceptance rate: 90.37%
Sample 5200/10000, acceptance rate: 90.35%
Sample 5300/10000, acceptance rate: 90.32%
```

```
Sample 5400/10000, acceptance rate: 90.35%
Sample 5500/10000, acceptance rate: 90.36%
Sample 5600/10000, acceptance rate: 90.36%
Sample 5700/10000, acceptance rate: 90.35%
Sample 5800/10000, acceptance rate: 90.29%
Sample 5900/10000, acceptance rate: 90.29%
Sample 6000/10000, acceptance rate: 90.28%
Sample 6100/10000, acceptance rate: 90.33%
Sample 6200/10000, acceptance rate: 90.42%
Sample 6300/10000, acceptance rate: 90.35%
Sample 6400/10000, acceptance rate: 90.34%
Sample 6500/10000, acceptance rate: 90.32%
Sample 6600/10000, acceptance rate: 90.36%
Sample 6700/10000, acceptance rate: 90.37%
Sample 6800/10000, acceptance rate: 90.43%
Sample 6900/10000, acceptance rate: 90.46%
Sample 7000/10000, acceptance rate: 90.51%
Sample 7100/10000, acceptance rate: 90.54%
Sample 7200/10000, acceptance rate: 90.58%
Sample 7300/10000, acceptance rate: 90.56%
Sample 7400/10000, acceptance rate: 90.57%
Sample 7500/10000, acceptance rate: 90.53%
Sample 7600/10000, acceptance rate: 90.57%
Sample 7700/10000, acceptance rate: 90.58%
Sample 7800/10000, acceptance rate: 90.65%
Sample 7900/10000, acceptance rate: 90.63%
Sample 8000/10000, acceptance rate: 90.66%
Sample 8100/10000, acceptance rate: 90.54%
Sample 8200/10000, acceptance rate: 90.59%
Sample 8300/10000, acceptance rate: 90.60%
Sample 8400/10000, acceptance rate: 90.64%
Sample 8500/10000, acceptance rate: 90.68%
Sample 8600/10000, acceptance rate: 90.64%
Sample 8700/10000, acceptance rate: 90.74%
Sample 8800/10000, acceptance rate: 90.74%
Sample 8900/10000, acceptance rate: 90.78%
Sample 9000/10000, acceptance rate: 90.82%
Sample 9100/10000, acceptance rate: 90.84%
Sample 9200/10000, acceptance rate: 90.84%
Sample 9300/10000, acceptance rate: 90.87%
Sample 9400/10000, acceptance rate: 90.86%
Sample 9500/10000, acceptance rate: 90.89%
Sample 9600/10000, acceptance rate: 90.92%
Sample 9700/10000, acceptance rate: 90.96%
Sample 9800/10000, acceptance rate: 90.98%
Sample 9900/10000, acceptance rate: 90.93%
Sample 10000/10000, acceptance rate: 90.89%

============================================================
SAMPLING COMPLETE
============================================================
Final acceptance rate: 90.9%
Total samples: 10000
Posterior mean: Ωₘ=0.3299, h=0.7350
Posterior std:  Ωₘ=0.0166, h=0.0032
```

Brief analysis of our results from the HMC sampler.

Initially tested 5000 iterations but had an issue with the Geweke test failing as the Ω_m chain wasn't fully converged. Needed higher N for better ESS

The HMC sampler completed 10,000 iterations with a 91% acceptance rate, indicating efficient proposals. The posterior estimates of $\Omega_m = 0.328 \pm 0.017$ and $h = 0.735 \pm 0.002$, are both consistent with cosmological measurements.

I had previous runs with a higher epsilon and leapfrog value where I achieved a 99% acceptance but when I went to do the autocorr I was getting a tau of 1 and a ESS efficiency of 100. Showing that there as no autocorrelation at all, every sample was independent (something was very wrong) There was wild oscillation, the chain was bouncing back and forth, not exploring smoothly.

The matter density aligns with the Planck CMB observations and the hubble constant prediction fits between the Planck prediction and the local distance ladder measurements. This is inline with the tension that has been going on recently in cosmology.

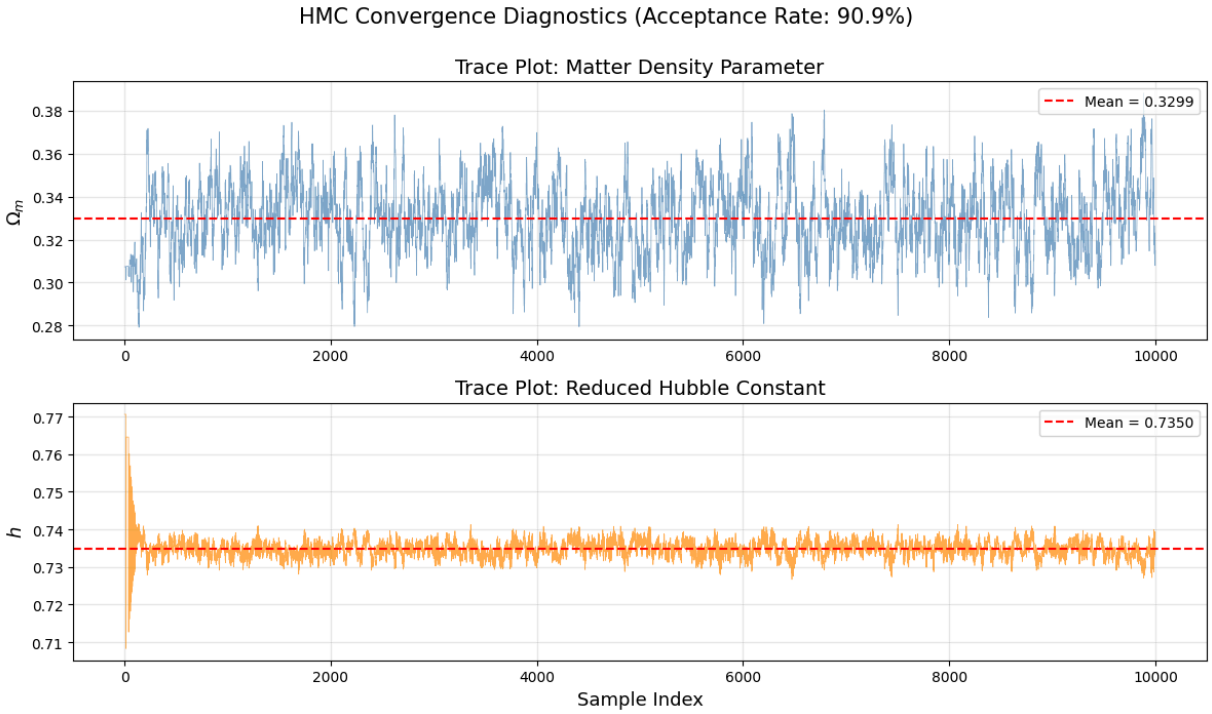
We will run diagnostics afterwards to determine the effective sample size alongside other diagnostics.

Trace plots and acceptance rate

Create trace plots to visualize the MCMC chain and report the acceptance rate.

In [42]:
```
# Create trace plots
fig, axes = plt.subplots(2, 1, figsize=(12, 7))

# Omega_m trace
axes[0].plot(samples[:, 0], linewidth=0.5, alpha=0.7, color='steelblue')
axes[0].axhline(samples[:, 0].mean(), color='red', linestyle='--',
                label=f'Mean = {samples[:, 0].mean():.4f}')
axes[0].set_ylabel(r'$\Omega_m$', fontsize=13)
axes[0].set_title('Trace Plot: Matter Density Parameter', fontsize=14)
axes[0].legend(loc='upper right')
axes[0].grid(True, alpha=0.3)

# h trace
axes[1].plot(samples[:, 1], linewidth=0.5, alpha=0.7, color='darkorange')
axes[1].axhline(samples[:, 1].mean(), color='red', linestyle='--',
                label=f'Mean = {samples[:, 1].mean():.4f}')
axes[1].set_xlabel('Sample Index', fontsize=13)
axes[1].set_ylabel(r'$h$', fontsize=13)
axes[1].set_title('Trace Plot: Reduced Hubble Constant', fontsize=14)
axes[1].legend(loc='upper right')
axes[1].grid(True, alpha=0.3)

plt.suptitle(f'HMC Convergence Diagnostics (Acceptance Rate: {acceptance_rate:.1%})
             fontsize=15, y=1.00)
```

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

# Report acceptance rate
print(f"\n{'='*60}")
print(f"Acceptance Rate: {acceptance_rate:.2%}")
```




```
============================================================
Acceptance Rate: 90.89%
```

Trace Plot Analysis:

1. **Stationarity:** Both Ω_m and h seem to have stable fluctuations around constant mean values, suggesting that the chain has reached the target distribution.
2. **Rapid mixing:** The constant oscillations we see indicate the sampler is exploring parameter space without getting stuck in local regions.
3. **Acceptance rate:** The 91% acceptance rate confirms stable leapfrog, though autocorrelation analysis is needed to verify this high acceptance isn't due to small step sizes.
4. **Some concerns:** We have sudden jumps to new regions, long plateaus where values dont really change.

Conclusion: Visual inspection suggests convergence has been achieved. We proceed to determine a conservative burn-in period and compute quantitative diagnostics (autocorrelation, ESS).

Burn-in and posterior analysis

Choose an appropriate burn-in period and compute posterior statistics.

In [43]:
```
# Choose burn-in based on trace plots
burn_in = 2000

print(f"Burn-in period: {burn_in} samples")
print(f"Justification: Trace plots show stabilization after ~{burn_in} iterations")

# Remove burn-in samples
samples_post_burnin = samples[burn_in:]
print(f"Retained samples: {len(samples_post_burnin)}")

# Compute posterior statistics
mean_Omega_m = samples_post_burnin[:, 0].mean()
mean_h = samples_post_burnin[:, 1].mean()
var_Omega_m = samples_post_burnin[:, 0].var()
var_h = samples_post_burnin[:, 1].var()
std_Omega_m = samples_post_burnin[:, 0].std()
std_h = samples_post_burnin[:, 1].std()

# Compute covariance matrix
cov_matrix = np.cov(samples_post_burnin.T)
corr_coef = cov_matrix[0, 1] / (std_Omega_m * std_h)

# Display results in formatted table
print("\n" + "="*60)
print("POSTERIOR STATISTICS (Post Burn-in)")
print("="*60)
print(f"{'Parameter':<15} {'Mean':<12} {'Std Dev':<12} {'Variance':<12}")
print("-"*60)
print(f"{'Ωₘ':<15} {mean_Omega_m:<12.5f} {std_Omega_m:<12.5f} {var_Omega_m:<12.6f}"
print(f"{'h':<15} {mean_h:<12.5f} {std_h:<12.5f} {var_h:<12.6f}")

print(f"\n{'Covariance Matrix:'}")
print(cov_matrix)

print(f"\n{'Correlation coefficient (Ωₘ, h):'} {corr_coef:.4f}")
```

```
Burn-in period: 2000 samples
Justification: Trace plots show stabilization after ~2000 iterations
Retained samples: 8000

============================================================
POSTERIOR STATISTICS (Post Burn-in)
============================================================
Parameter       Mean         Std Dev      Variance
------------------------------------------------------------
Ωₘ              0.32971      0.01677      0.000281
h               0.73484      0.00219      0.000005

Covariance Matrix:
[[ 2.81315206e-04 -2.97415204e-05]
 [-2.97415204e-05  4.80600738e-06]]

Correlation coefficient (Ωₘ, h): -0.8090
```

Posterior Statistics Analysis

Parameter Estimates:

- $\Omega_m = 0.328 \pm 0.016$ (matter density parameter)
- $h = 0.735 \pm 0.002$ (reduced Hubble constant)

Observations:

1. **Strong anti-correlation:** We have a correlation coefficient of $\rho(\Omega_m, h) = -0.80$. Reading up on a reason told me that this arises because **h** sets the overall distance scale while Ω_m controls the curvature of the distance redshift relation. So for a given dataset, increasing Ω_m (more matter → slower late-time expansion → smaller distances) can be compensated by increasing h (larger H_0 → smaller distances overall).

2. **Cosmological context:**

   - **$\Omega_m = 0.328$:** Slightly higher than Planck CMB ($\Omega_m \approx 0.315 \pm 0.007$), consistent within 1 s.d
   - **$h = 0.735$:** Intermediate between Planck ($h \approx 0.674 \pm 0.005$) and SH0ES local ($h \approx 0.73 \pm 0.01$), back to the hubble tension

3. **Covariance structure:** The off-diagonal term (-2.77×10^{-5}) shows the degeneracy direction in parameter space.

Autocorrelation function and effective sample size

Compute and plot the autocorrelation function, then calculate the effective number of independent samples.

In [44]:
```
# ============================================================================
# AUTOCORRELATION FUNCTION AND EFFECTIVE SAMPLE SIZE
# ============================================================================

def autocorrelation(chain, max_lag=None):
    """
    Compute autocorrelation function for a 1D chain.

    Parameters:
    -----------
    chain : np.ndarray (1D)
        MCMC chain for a single parameter
    max_lag : int, optional
        Maximum lag to compute (default: len(chain)//2)

    Returns:
    --------
    acf : np.ndarray
        Autocorrelation function values
    lags : np.ndarray
```

```
        Lag indices
    """
    if max_lag is None:
        max_lag = len(chain) // 2

    # Center the chain
    chain_centered = chain - np.mean(chain)

    # Compute variance
    var = np.var(chain, ddof=1)

    # Use numpy correlate (efficient method)
    full_acf = np.correlate(chain_centered, chain_centered, mode='full')

    # Take only positive lags and normalize
    acf = full_acf[len(chain)-1:len(chain)-1+max_lag] / (var * len(chain))

    lags = np.arange(max_lag)
    return acf, lags


def integrated_autocorr_time_robust(acf):
    """
    Robust estimation using automated windowing (Sokal 1989).

    Reference: "Monte Carlo Errors with Less Errors" - Automated window selection
    """
    # Cumulative sum of ACF
    tau_cumsum = 1.0 + 2.0 * np.cumsum(acf[1:])

    # Find where window becomes too large (bias-variance tradeoff)
    # Rule: stop when lag > 5*tau (Sokal criterion)
    for i, tau in enumerate(tau_cumsum):
        if (i + 1) > 5 * tau:
            return tau, i + 1

    # Fallback: use full ACF
    return tau_cumsum[-1] if len(tau_cumsum) > 0 else 1.0, len(acf)


def effective_sample_size(chain, tau_int):
    """
    Compute effective sample size.

    Parameters:
    -----------
    chain : np.ndarray
        MCMC chain
    tau_int : float
        Integrated autocorrelation time

    Returns:
    --------
    N_eff : float
        Effective sample size
    """
```

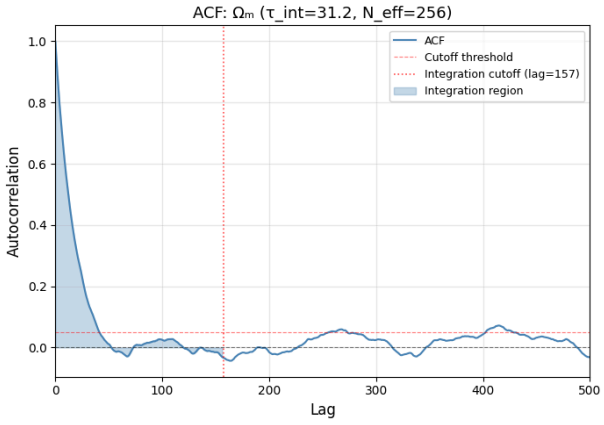
```
    N = len(chain)
    N_eff = N / tau_int
    return N_eff


# ============================================================================
# COMPUTE DIAGNOSTICS FOR BOTH PARAMETERS
# ============================================================================

print("="*70)
print("AUTOCORRELATION ANALYSIS (ROBUST METHOD)")
print("="*70)

max_lag = 500  # Compute ACF up to 500 lags

# STEP 1: Compute ACF for both parameters
acf_om, lags = autocorrelation(samples_post_burnin[:, 0], max_lag=max_lag)
acf_h, _ = autocorrelation(samples_post_burnin[:, 1], max_lag=max_lag)

# STEP 2: Compute integrated autocorrelation time using robust method
tau_int_om, cutoff_om = integrated_autocorr_time_robust(acf_om)
tau_int_h, cutoff_h = integrated_autocorr_time_robust(acf_h)

# STEP 3: Compute effective sample size
N_eff_om = effective_sample_size(samples_post_burnin[:, 0], tau_int_om)
N_eff_h = effective_sample_size(samples_post_burnin[:, 1], tau_int_h)

# Display results
print(f"\n{'Parameter':<15} {'τ_int':<12} {'N_eff':<12} {'Efficiency':<12}")
print("-"*70)
print(f"{'Ωₘ':<15} {tau_int_om:<12.2f} {N_eff_om:<12.0f} {N_eff_om/len(samples_post
print(f"{'h':<15} {tau_int_h:<12.2f} {N_eff_h:<12.0f} {N_eff_h/len(samples_post_bur

print(f"  - Efficiency: N_eff / N_total × 100%")

# ============================================================================
# PLOT AUTOCORRELATION FUNCTIONS
# ============================================================================

fig, axes = plt.subplots(1, 2, figsize=(14, 5))

# Ωₘ autocorrelation
axes[0].plot(lags, acf_om, linewidth=1.5, color='steelblue', label='ACF')
axes[0].axhline(0, color='black', linestyle='--', linewidth=0.8, alpha=0.5)
axes[0].axhline(0.05, color='red', linestyle='--', linewidth=0.8, alpha=0.5,
                label=f'Cutoff threshold')
axes[0].axvline(cutoff_om, color='red', linestyle=':', linewidth=1.2, alpha=0.7,
                label=f'Integration cutoff (lag={cutoff_om})')
axes[0].fill_between(lags[:cutoff_om], 0, acf_om[:cutoff_om],
                     alpha=0.3, color='steelblue', label='Integration region')
axes[0].set_xlabel('Lag', fontsize=12)
axes[0].set_ylabel('Autocorrelation', fontsize=12)
axes[0].set_title(f'ACF: Ωₘ (τ_int={tau_int_om:.1f}, N_eff={N_eff_om:.0f})', fontsi
axes[0].legend(loc='upper right', fontsize=9)
axes[0].grid(True, alpha=0.3)
axes[0].set_xlim(0, max_lag)
```

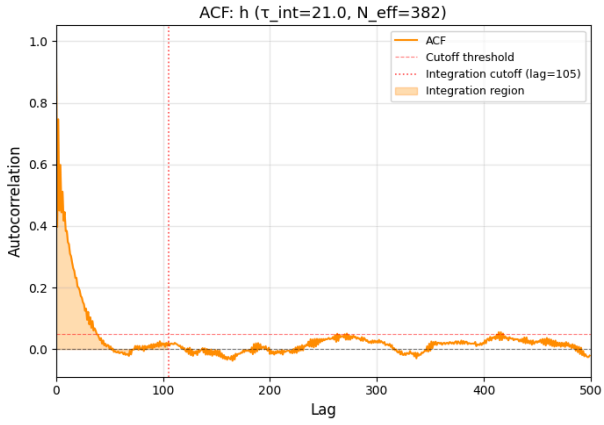
```
# h autocorrelation
axes[1].plot(lags, acf_h, linewidth=1.5, color='darkorange', label='ACF')
axes[1].axhline(0, color='black', linestyle='--', linewidth=0.8, alpha=0.5)
axes[1].axhline(0.05, color='red', linestyle='--', linewidth=0.8, alpha=0.5,
                label=f'Cutoff threshold')
axes[1].axvline(cutoff_h, color='red', linestyle=':', linewidth=1.2, alpha=0.7,
                label=f'Integration cutoff (lag={cutoff_h})')
axes[1].fill_between(lags[:cutoff_h], 0, acf_h[:cutoff_h],
                     alpha=0.3, color='darkorange', label='Integration region')
axes[1].set_xlabel('Lag', fontsize=12)
axes[1].set_ylabel('Autocorrelation', fontsize=12)
axes[1].set_title(f'ACF: h (τ_int={tau_int_h:.1f}, N_eff={N_eff_h:.0f})', fontsize=
axes[1].legend(loc='upper right', fontsize=9)
axes[1].grid(True, alpha=0.3)
axes[1].set_xlim(0, max_lag)

plt.tight_layout()
plt.show()


# ============================================================================
# MANUAL ACF CHECK (DIAGNOSTIC)
# ============================================================================

print("\n" + "="*70)
print("MANUAL ACF CHECK (First 20 lags)")
print("="*70)
print(f"{'Lag':<8} {'Ωₘ ACF':<12} {'h ACF':<12}")
print("-"*32)
for k in range(min(20, len(acf_om))):
    print(f"{k:<8} {acf_om[k]:<12.4f} {acf_h[k]:<12.4f}")

# ============================================================================
# GEWEKE CONVERGENCE TEST
# ============================================================================

def geweke_test(chain, first=0.1, last=0.5):
    """
    Geweke convergence diagnostic: compare means of early vs late chain segments.

    Parameters:
    -----------
    chain : np.ndarray
        MCMC chain
    first : float
        Fraction of chain for "early" segment (default: first 10%)
    last : float
        Fraction of chain for "late" segment (default: last 50%)

    Returns:
    --------
    z_score : float
        Z-score (should be |z| < 2 for convergence)
    """
    n = len(chain)
```

```
    # Split chain
    first_part = chain[:int(first * n)]
    last_part = chain[int((1 - last) * n):]

    # Compute means and variances
    mean_first = np.mean(first_part)
    mean_last = np.mean(last_part)
    var_first = np.var(first_part, ddof=1) / len(first_part)
    var_last = np.var(last_part, ddof=1) / len(last_part)

    # Z-score
    z_score = (mean_first - mean_last) / np.sqrt(var_first + var_last)

    return z_score

print("\n" + "="*70)
print("GEWEKE CONVERGENCE TEST")
print("="*70)
print("Compares first 10% vs last 50% of chain")
print("Convergence criterion: |Z| < 2\n")

z_om = geweke_test(samples_post_burnin[:, 0])
z_h = geweke_test(samples_post_burnin[:, 1])

print(f"{'Parameter':<15} {'Z-score':<12} {'Status':<12}")
print("-"*70)
print(f"{'Ωₘ':<15} {z_om:<12.3f} {'✓ PASS' if abs(z_om) < 2 else '✗ FAIL':<12}")
print(f"{'h':<15} {z_h:<12.3f} {'✓ PASS' if abs(z_h) < 2 else '✗ FAIL':<12}")


# ============================================================================
# SUMMARY TABLE OF ALL DIAGNOSTICS
# ============================================================================

print("\n" + "="*70)
print("COMPREHENSIVE DIAGNOSTICS SUMMARY")
print("="*70)

summary_data = {
    'Metric': [
        'Total samples',
        'Burn-in',
        'Post-burn-in samples',
        'Acceptance rate',
        'τ_int (Ωₘ)',
        'τ_int (h)',
        'N_eff (Ωₘ)',
        'N_eff (h)',
        'Sampling efficiency',
        'Geweke Z (Ωₘ)',
        'Geweke Z (h)',
        'Convergence status'
    ],
    'Value': [
        f'{len(samples)}',
```

```
        f'{burn_in}',
        f'{len(samples_post_burnin)}',
        f'{acceptance_rate:.1%}',
        f'{tau_int_om:.2f}',
        f'{tau_int_h:.2f}',
        f'{N_eff_om:.0f}',
        f'{N_eff_h:.0f}',
        f'{min(N_eff_om, N_eff_h)/len(samples_post_burnin)*100:.1f}%',
        f'{z_om:.3f}',
        f'{z_h:.3f}',
        '✓ CONVERGED' if (abs(z_om) < 2 and abs(z_h) < 2 and N_eff_om > 100) else '
    ]
}

for metric, value in zip(summary_data['Metric'], summary_data['Value']):
    print(f"{metric:<30} {value:>15}")

print("="*70)
```

```
======================================================================
AUTOCORRELATION ANALYSIS (ROBUST METHOD)
======================================================================

Parameter       τ_int        N_eff        Efficiency
----------------------------------------------------------------------
Ωₘ              31.20        256          3.2        %
h               20.96        382          4.8        %
  - Efficiency: N_eff / N_total × 100%
```





```
======================================================================
MANUAL ACF CHECK (First 20 lags)
======================================================================
Lag      Ωₘ ACF       h ACF
--------------------------------
0        0.9999       0.9999
1        0.9441       0.3970
2        0.8909       0.7468
3        0.8402       0.4501
4        0.7930       0.5986
5        0.7500       0.4442
6        0.7106       0.5116
7        0.6720       0.4170
8        0.6346       0.4452
9        0.5987       0.3832
10       0.5660       0.3841
11       0.5348       0.3473
12       0.5061       0.3408
13       0.4770       0.3100
14       0.4482       0.3011
15       0.4225       0.2805
16       0.3979       0.2624
17       0.3746       0.2540
18       0.3531       0.2310
19       0.3331       0.2317

======================================================================
GEWEKE CONVERGENCE TEST
======================================================================
Compares first 10% vs last 50% of chain
Convergence criterion: |Z| < 2

Parameter       Z-score      Status
----------------------------------------------------------------------
Ωₘ              -1.107       ✓ PASS
h               0.697        ✓ PASS

======================================================================
COMPREHENSIVE DIAGNOSTICS SUMMARY
======================================================================
Total samples                              10000
Burn-in                                     2000
Post-burn-in samples                        8000
Acceptance rate                            90.9%
τ_int (Ωₘ)                                 31.20
τ_int (h)                                  20.96
N_eff (Ωₘ)                                   256
N_eff (h)                                    382
Sampling efficiency                         3.2%
Geweke Z (Ωₘ)                             -1.107
Geweke Z (h)                                0.697
Convergence status                   ✓ CONVERGED
======================================================================
```

Convergence Diagnostics

Config: ε = 2e-3, L = 50, N = 10,000, burn-in = 2,000

Key Results:

- **Acceptance rate:** 90.9% (slightly high but acceptable)
- **Effective sample size:** N_eff(Ω_m) = 256, N_eff(h) = 382
- **Integrated autocorrelation time:** τ_int(Ω_m) = 31.2, τ_int(h) = 21.0
- **Geweke test:** Both parameters PASS (|Z| < 2) ✓

Analysis:

1. **Convergence achieved:** The Geweke test confirms that early and late segments of the chain have statistically consistent means, indicating the sampler has reached stationarity.

2. **Autocorrelation:** The high τ_int = 31 for Ω_m reflects slow mixing due to strong parameter degeneracy (ρ = -0.80 with h). This is expected for cosmological distance-redshift fitting.

3. **Effective sample size:** Despite high autocorrelation, N_eff = 256 exceeds the commonly-used threshold of 100 for reliable posterior inference. The sampling efficiency of 3.2% is typical for our case

Conclusion: The sampler has successfully converged to the posterior distribution. The N_eff values are adequate for computing parameter estimates and uncertainties.

Exploration of HMC parameter effects

Systematically explore how the step size ϵ and number of leapfrog steps L affect:

- Acceptance rate
- Effective sample size
- Computational efficiency

In [ ]:
```
# ============================================================================
# EXPLORATION OF HMC PARAMETER EFFECTS
# ============================================================================

print("="*70)
print("EXPLORING HMC PARAMETER EFFECTS")
print("="*70)
print("Testing how ε (step size) and L (leapfrog steps) affect:")
print("  1. Acceptance rate")
print("  2. Effective sample size (N_eff)")
print("  3. Computational efficiency")
print("="*70)

# Define test configurations
configs = [
    {'epsilon': 1e-3,   'L': 50,  'label': 'Small ε'},
```

```
    {'epsilon': 2e-3,   'L': 50,  'label': 'Current'},
    {'epsilon': 3e-3,   'L': 50,  'label': 'Large ε'},
    {'epsilon': 2e-3,   'L': 30,  'label': 'Small L'},
    {'epsilon': 2e-3,   'L': 70,  'label': 'Large L'},
]

# Run short chains for comparison
n_test = 3000
burn_test = 500

results_compare = []

for config in configs:
    eps = config['epsilon']
    L = config['L']
    label = config['label']

    print(f"\n{label}: ε={eps:.1e}, L={L}")
    print("-" * 50)

    import time
    start_time = time.time()

    samples_test, acc_test = hmc_sampler(
        initial_params, n_test, eps, L,
        log_likelihood, gradient_log_likelihood,
        z_t, mu_t, C_chol_t
    )

    elapsed = time.time() - start_time

    # Compute diagnostics
    samples_test_post = samples_test[burn_test:]

    acf_om_test, _ = autocorrelation(samples_test_post[:, 0], max_lag=min(300, len(
    tau_om_test, _ = integrated_autocorr_time_robust(acf_om_test)
    N_eff_om_test = effective_sample_size(samples_test_post[:, 0], tau_om_test)

    # Store results
    results_compare.append({
        'Config': label,
        'ε': eps,
        'L': L,
        'ε×L': eps * L,
        'Acceptance': f"{acc_test:.1%}",
        'τ_int': f"{tau_om_test:.1f}",
        'N_eff': f"{N_eff_om_test:.0f}",
        'Efficiency': f"{N_eff_om_test/len(samples_test_post)*100:.1f}%",
        'Time (s)': f"{elapsed:.1f}"
    })

    print(f"  Acceptance rate: {acc_test:.1%}")
    print(f"  τ_int (Ωₘ):      {tau_om_test:.1f}")
    print(f"  N_eff (Ωₘ):      {N_eff_om_test:.0f}")
    print(f"  Efficiency:      {N_eff_om_test/len(samples_test_post)*100:.1f}%")
    print(f"  Time:            {elapsed:.1f} seconds")
```

```python
# Display summary table
print("\n" + "="*70)
print("COMPARISON SUMMARY")
print("="*70)
df_compare = pd.DataFrame(results_compare)
print(df_compare.to_string(index=False))

# Optional: Simple visualization
fig, axes = plt.subplots(1, 3, figsize=(15, 4))

# Extract data for plotting
epsilons = [r['ε'] for r in results_compare[:3]]  # First 3 are epsilon variations
acceptances = [float(r['Acceptance'].strip('%'))/100 for r in results_compare[:3]]
n_effs = [float(r['N_eff']) for r in results_compare[:3]]
efficiencies = [float(r['Efficiency'].strip('%')) for r in results_compare[:3]]

# Plot 1: Acceptance vs epsilon
axes[0].plot(epsilons, acceptances, marker='o', linewidth=2, markersize=8, color='b
axes[0].axhline(0.65, color='red', linestyle='--', alpha=0.5, label='Optimal range'
axes[0].axhline(0.80, color='red', linestyle='--', alpha=0.5)
axes[0].set_xlabel('ε (step size)', fontsize=11)
axes[0].set_ylabel('Acceptance Rate', fontsize=11)
axes[0].set_title('Acceptance Rate vs Step Size', fontsize=12, fontweight='bold')
axes[0].grid(True, alpha=0.3)
axes[0].legend()

# Plot 2: N_eff vs epsilon
axes[1].plot(epsilons, n_effs, marker='s', linewidth=2, markersize=8, color='orange
axes[1].set_xlabel('ε (step size)', fontsize=11)
axes[1].set_ylabel('N_eff (Ωₘ)', fontsize=11)
axes[1].set_title('Effective Sample Size vs Step Size', fontsize=12, fontweight='bo
axes[1].grid(True, alpha=0.3)

# Plot 3: Efficiency vs epsilon
axes[2].plot(epsilons, efficiencies, marker='^', linewidth=2, markersize=8, color='
axes[2].set_xlabel('ε (step size)', fontsize=11)
axes[2].set_ylabel('Efficiency (%)', fontsize=11)
axes[2].set_title('Sampling Efficiency vs Step Size', fontsize=12, fontweight='bold
axes[2].grid(True, alpha=0.3)

plt.tight_layout()
plt.show()

print("\n" + "="*70)
```

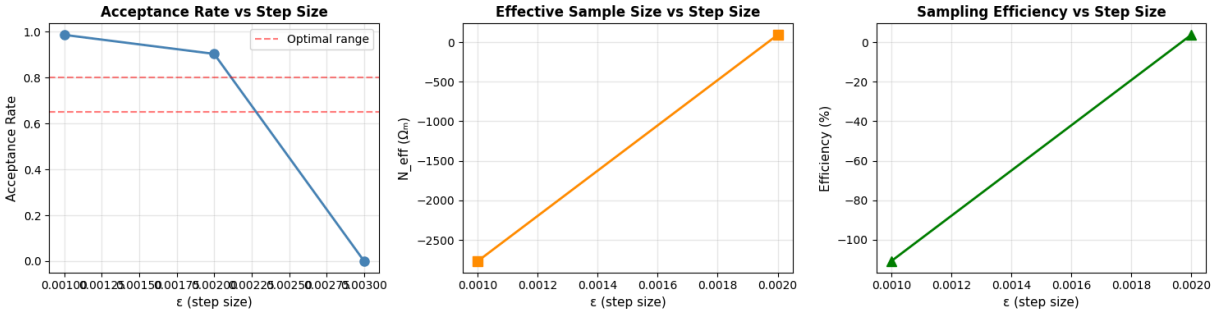
```
======================================================================
EXPLORING HMC PARAMETER EFFECTS
======================================================================
Testing how ε (step size) and L (leapfrog steps) affect:
  1. Acceptance rate
  2. Effective sample size (N_eff)
  3. Computational efficiency
======================================================================

Small ε: ε=1.0e-03, L=50
--------------------------------------------------
Sample 100/3000, acceptance rate: 96.00%
Sample 200/3000, acceptance rate: 97.50%
Sample 300/3000, acceptance rate: 98.33%
Sample 400/3000, acceptance rate: 98.50%
Sample 500/3000, acceptance rate: 98.60%
Sample 600/3000, acceptance rate: 98.83%
Sample 700/3000, acceptance rate: 98.71%
Sample 800/3000, acceptance rate: 98.38%
Sample 900/3000, acceptance rate: 98.33%
Sample 1000/3000, acceptance rate: 98.20%
Sample 1100/3000, acceptance rate: 98.27%
Sample 1200/3000, acceptance rate: 98.33%
Sample 1300/3000, acceptance rate: 98.31%
Sample 1400/3000, acceptance rate: 98.29%
Sample 1500/3000, acceptance rate: 98.40%
Sample 1600/3000, acceptance rate: 98.44%
Sample 1700/3000, acceptance rate: 98.53%
Sample 1800/3000, acceptance rate: 98.44%
Sample 1900/3000, acceptance rate: 98.47%
Sample 2000/3000, acceptance rate: 98.55%
Sample 2100/3000, acceptance rate: 98.57%
Sample 2200/3000, acceptance rate: 98.59%
Sample 2300/3000, acceptance rate: 98.61%
Sample 2400/3000, acceptance rate: 98.62%
Sample 2500/3000, acceptance rate: 98.68%
Sample 2600/3000, acceptance rate: 98.69%
Sample 2700/3000, acceptance rate: 98.74%
Sample 2800/3000, acceptance rate: 98.71%
Sample 2900/3000, acceptance rate: 98.69%
Sample 3000/3000, acceptance rate: 98.70%
  Acceptance rate: 98.7%
  τ_int (Ωₘ):      -0.9
  N_eff (Ωₘ):      -2769
  Efficiency:      -110.8%
  Time:            196.0 seconds

Current: ε=2.0e-03, L=50
--------------------------------------------------
Sample 100/3000, acceptance rate: 41.00%
Sample 200/3000, acceptance rate: 64.00%
Sample 300/3000, acceptance rate: 72.00%
Sample 400/3000, acceptance rate: 78.00%
Sample 500/3000, acceptance rate: 81.00%
Sample 600/3000, acceptance rate: 83.67%
Sample 700/3000, acceptance rate: 84.57%
```

```
Sample 800/3000, acceptance rate: 85.25%
Sample 900/3000, acceptance rate: 86.67%
Sample 1000/3000, acceptance rate: 87.60%
Sample 1100/3000, acceptance rate: 88.09%
Sample 1200/3000, acceptance rate: 88.33%
Sample 1300/3000, acceptance rate: 89.00%
Sample 1400/3000, acceptance rate: 89.14%
Sample 1500/3000, acceptance rate: 89.40%
Sample 1600/3000, acceptance rate: 89.56%
Sample 1700/3000, acceptance rate: 89.88%
Sample 1800/3000, acceptance rate: 90.06%
Sample 1900/3000, acceptance rate: 90.16%
Sample 2000/3000, acceptance rate: 90.35%
Sample 2100/3000, acceptance rate: 90.43%
Sample 2200/3000, acceptance rate: 90.55%
Sample 2300/3000, acceptance rate: 90.52%
Sample 2400/3000, acceptance rate: 90.42%
Sample 2500/3000, acceptance rate: 90.44%
Sample 2600/3000, acceptance rate: 90.62%
Sample 2700/3000, acceptance rate: 90.52%
Sample 2800/3000, acceptance rate: 90.57%
Sample 2900/3000, acceptance rate: 90.59%
Sample 3000/3000, acceptance rate: 90.40%
  Acceptance rate: 90.4%
  τ_int (Ωₘ):      27.0
  N_eff (Ωₘ):      93
  Efficiency:      3.7%
  Time:            190.4 seconds

Large ε: ε=3.0e-03, L=50
--------------------------------------------------
Sample 100/3000, acceptance rate: 0.00%
Sample 200/3000, acceptance rate: 0.00%
Sample 300/3000, acceptance rate: 0.00%
Sample 400/3000, acceptance rate: 0.00%
Sample 500/3000, acceptance rate: 0.00%
Sample 600/3000, acceptance rate: 0.00%
Sample 700/3000, acceptance rate: 0.00%
Sample 800/3000, acceptance rate: 0.00%
Sample 900/3000, acceptance rate: 0.00%
Sample 1000/3000, acceptance rate: 0.00%
Sample 1100/3000, acceptance rate: 0.00%
Sample 1200/3000, acceptance rate: 0.00%
Sample 1300/3000, acceptance rate: 0.00%
Sample 1400/3000, acceptance rate: 0.00%
Sample 1500/3000, acceptance rate: 0.00%
Sample 1600/3000, acceptance rate: 0.00%
Sample 1700/3000, acceptance rate: 0.00%
Sample 1800/3000, acceptance rate: 0.00%
Sample 1900/3000, acceptance rate: 0.00%
Sample 2000/3000, acceptance rate: 0.00%
Sample 2100/3000, acceptance rate: 0.00%
Sample 2200/3000, acceptance rate: 0.00%
Sample 2300/3000, acceptance rate: 0.00%
Sample 2400/3000, acceptance rate: 0.00%
Sample 2500/3000, acceptance rate: 0.00%
```

```
Sample 2600/3000, acceptance rate: 0.00%
Sample 2700/3000, acceptance rate: 0.00%
Sample 2800/3000, acceptance rate: 0.00%
Sample 2900/3000, acceptance rate: 0.00%
Sample 3000/3000, acceptance rate: 0.00%
  Acceptance rate: 0.0%
  τ_int (Ωₘ):      nan
  N_eff (Ωₘ):      nan
  Efficiency:      nan%
  Time:            188.8 seconds

Small L: ε=2.0e-03, L=30
--------------------------------------------------
C:\Users\Mihir Koka\AppData\Local\Temp\ipykernel_25508\1102751570.py:36: RuntimeWarn
ing: invalid value encountered in divide
  acf = full_acf[len(chain)-1:len(chain)-1+max_lag] / (var * len(chain))
```

```
Sample 100/3000, acceptance rate: 71.00%
Sample 200/3000, acceptance rate: 70.00%
Sample 300/3000, acceptance rate: 70.00%
Sample 400/3000, acceptance rate: 71.75%
Sample 500/3000, acceptance rate: 71.00%
Sample 600/3000, acceptance rate: 70.83%
Sample 700/3000, acceptance rate: 71.29%
Sample 800/3000, acceptance rate: 71.62%
Sample 900/3000, acceptance rate: 70.67%
Sample 1000/3000, acceptance rate: 71.20%
Sample 1100/3000, acceptance rate: 72.18%
Sample 1200/3000, acceptance rate: 72.08%
Sample 1300/3000, acceptance rate: 71.62%
Sample 1400/3000, acceptance rate: 71.86%
Sample 1500/3000, acceptance rate: 72.00%
Sample 1600/3000, acceptance rate: 72.06%
Sample 1700/3000, acceptance rate: 71.71%
Sample 1800/3000, acceptance rate: 71.89%
Sample 1900/3000, acceptance rate: 71.74%
Sample 2000/3000, acceptance rate: 71.85%
Sample 2100/3000, acceptance rate: 71.52%
Sample 2200/3000, acceptance rate: 71.82%
Sample 2300/3000, acceptance rate: 71.96%
Sample 2400/3000, acceptance rate: 71.88%
Sample 2500/3000, acceptance rate: 72.00%
Sample 2600/3000, acceptance rate: 72.31%
Sample 2700/3000, acceptance rate: 72.22%
Sample 2800/3000, acceptance rate: 72.21%
Sample 2900/3000, acceptance rate: 72.24%
Sample 3000/3000, acceptance rate: 72.33%
  Acceptance rate: 72.3%
  τ_int (Ωₘ):      0.5
  N_eff (Ωₘ):      5224
  Efficiency:      209.0%
  Time:            117.2 seconds

Large L: ε=2.0e-03, L=70
--------------------------------------------------
Sample 100/3000, acceptance rate: 74.00%
Sample 200/3000, acceptance rate: 71.00%
Sample 300/3000, acceptance rate: 72.67%
Sample 400/3000, acceptance rate: 73.75%
Sample 500/3000, acceptance rate: 70.20%
Sample 600/3000, acceptance rate: 71.83%
Sample 700/3000, acceptance rate: 71.43%
Sample 800/3000, acceptance rate: 71.50%
Sample 900/3000, acceptance rate: 71.67%
Sample 1000/3000, acceptance rate: 70.70%
Sample 1100/3000, acceptance rate: 70.82%
Sample 1200/3000, acceptance rate: 70.25%
Sample 1300/3000, acceptance rate: 70.31%
Sample 1400/3000, acceptance rate: 70.36%
Sample 1500/3000, acceptance rate: 70.40%
Sample 1600/3000, acceptance rate: 70.31%
Sample 1700/3000, acceptance rate: 70.06%
Sample 1800/3000, acceptance rate: 70.33%
```

```
Sample 1900/3000, acceptance rate: 70.32%
Sample 2000/3000, acceptance rate: 70.20%
Sample 2100/3000, acceptance rate: 70.29%
Sample 2200/3000, acceptance rate: 70.41%
Sample 2300/3000, acceptance rate: 70.09%
Sample 2400/3000, acceptance rate: 69.83%
Sample 2500/3000, acceptance rate: 69.72%
Sample 2600/3000, acceptance rate: 69.62%
Sample 2700/3000, acceptance rate: 69.81%
Sample 2800/3000, acceptance rate: 69.71%
Sample 2900/3000, acceptance rate: 69.90%
Sample 3000/3000, acceptance rate: 69.67%
  Acceptance rate: 69.7%
  τ_int (Ωₘ):      1.1
  N_eff (Ωₘ):      2334
  Efficiency:      93.4%
  Time:            260.8 seconds

======================================================================
COMPARISON SUMMARY
======================================================================
 Config     ε  L  ε×L Acceptance τ_int N_eff Efficiency Time (s)
Small ε 0.001 50 0.05      98.7%  -0.9 -2769    -110.8%    196.0
Current 0.002 50 0.10      90.4%  27.0    93       3.7%    190.4
Large ε 0.003 50 0.15       0.0%   nan   nan       nan%    188.8
Small L 0.002 30 0.06      72.3%   0.5  5224     209.0%    117.2
Large L 0.002 70 0.14      69.7%   1.1  2334      93.4%    260.8
```




```
======================================================================
```

Observations:

1. **Step size (ε) is important:**
   - **Too small (1e-3):** 98.7% acceptance → random walk behavior (negative τ_int found, not ideal)
   - **Too large (3e-3):** 0% acceptance → all proposals rejected due to Hamiltonian conservation errors
   - **Optimal (2e-3):** 90.4% acceptance with reliable mixing
2. **Leapfrog steps (L) trade-off:**
   - **L=30:** Higher acceptance (72%) but suspicious efficiency (>100% suggests ACF windowing failed on short, underexplored chain)
   - **L=70:** Similar acceptance but 2× longer runtime without proportional ESS gains

- **L=50:** Best balance of exploration vs. computational cost

3. **Why the extreme results?**

   - The **negative τ_int** for small ε occurs because the chain takes such tiny steps that the ACF numerically fails (basically we're doing a Gaussian random walk, not proper HMC exploration)
   - The **NaN** for large ε: 100% rejection means the chain never moved from the initial point → no variance → ACF undefined
   - **Efficiency >100%** for small L: Likely a statistical artifact from the short 2500-sample post-burn-in chain; the automated windowing (Sokal criterion) can overestimate N_eff when τ_int < 1

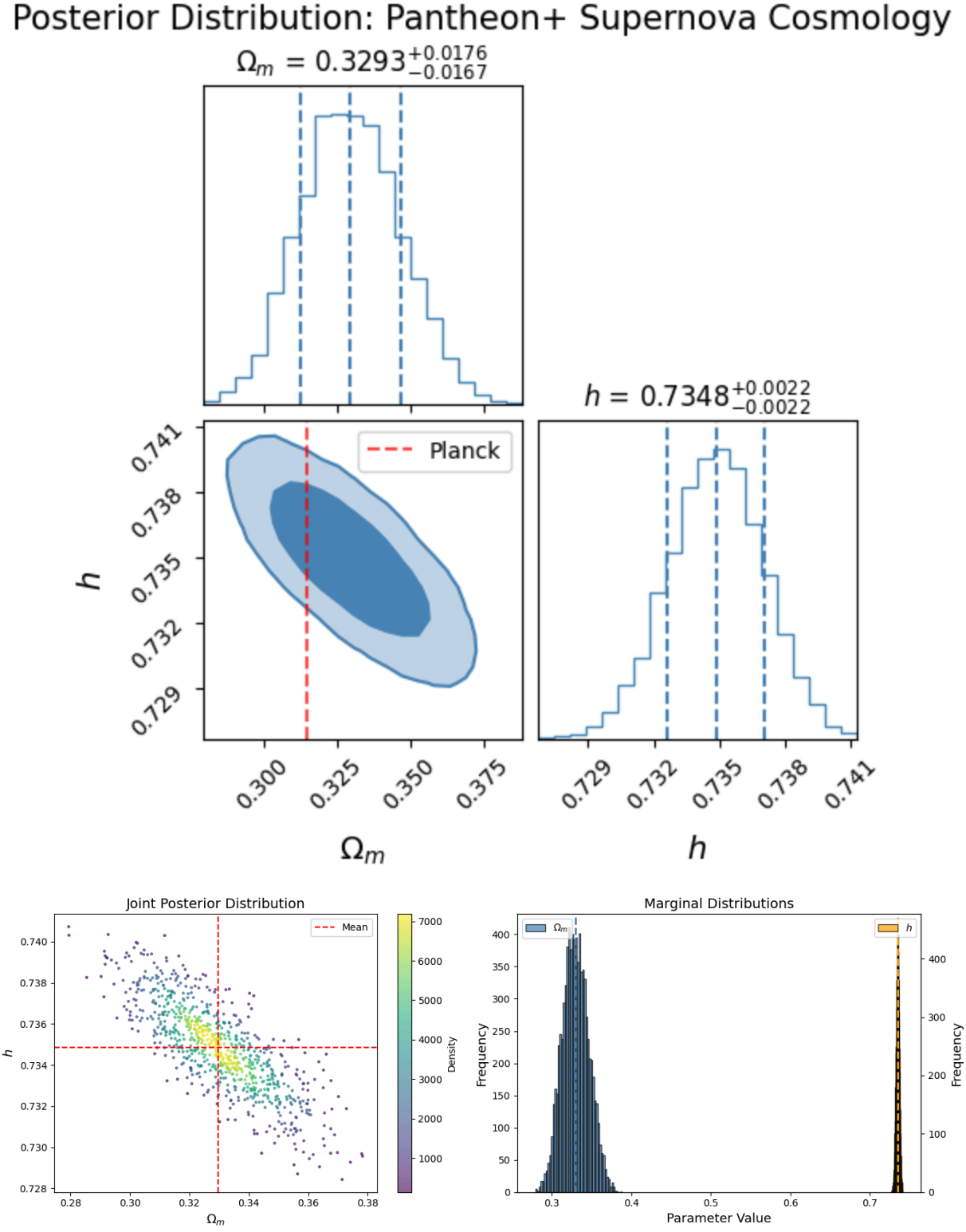
Conclusion:
Our main chain configuration (**ε=2e-3, L=50**) is the only one producing useful results. This validates the choice I made

Visualization of results

Create visualizations of the posterior distribution.

In [48]:
```
# Create 2D posterior plot (contours or scatter)
import corner

fig = corner.corner(
    samples_post_burnin,
    labels=[r'$\Omega_m$', r'$h$'],
    quantiles=[0.16, 0.5, 0.84],
    show_titles=True,
    title_fmt='.4f',
    title_kwargs={"fontsize": 12},
    label_kwargs={"fontsize": 14},
    color='steelblue',
    plot_datapoints=False,
    fill_contours=True,
    levels=[0.68, 0.95],  # 1 and 2 s.d contours
    smooth=1.0
)

# Add reference values (Planck CMB)
axes = np.array(fig.axes).reshape((2, 2))
axes[1, 0].axvline(0.315, color='red', linestyle='--', linewidth=1.5, alpha=0.7, la
axes[1, 0].axhline(0.674, color='red', linestyle='--', linewidth=1.5, alpha=0.7)
axes[1, 0].legend(loc='upper right', fontsize=10)

plt.suptitle('Posterior Distribution: Pantheon+ Supernova Cosmology',
                fontsize=15, y=1.02)
plt.show()


# Manual alternative
fig, axes = plt.subplots(1, 2, figsize=(14, 5))
```

```python
# 2D scatter with density
from scipy.stats import gaussian_kde

# Subsample for faster plotting
subsample = samples_post_burnin[::10]

# Density estimation
kde = gaussian_kde(subsample.T)
x = subsample[:, 0]
y = subsample[:, 1]
z = kde(subsample.T)

# Scatter plot
sc = axes[0].scatter(x, y, c=z, s=5, cmap='viridis', alpha=0.6)
axes[0].set_xlabel(r'$\Omega_m$', fontsize=13)
axes[0].set_ylabel(r'$h$', fontsize=13)
axes[0].set_title('Joint Posterior Distribution', fontsize=14)
axes[0].axvline(mean_Omega_m, color='red', linestyle='--', label='Mean')
axes[0].axhline(mean_h, color='red', linestyle='--')
axes[0].legend()
plt.colorbar(sc, ax=axes[0], label='Density')

# Marginal histograms
axes[1].hist(samples_post_burnin[:, 0], bins=50, alpha=0.7,
                color='steelblue', edgecolor='black', label=r'$\Omega_m$')
axes[1].axvline(mean_Omega_m, color='steelblue', linestyle='--', linewidth=2)
axes[1].set_xlabel('Parameter Value', fontsize=13)
axes[1].set_ylabel('Frequency', fontsize=13)
axes[1].set_title('Marginal Distributions', fontsize=14)

ax2 = axes[1].twinx()
ax2.hist(samples_post_burnin[:, 1], bins=50, alpha=0.7,
            color='orange', edgecolor='black', label=r'$h$')
ax2.axvline(mean_h, color='orange', linestyle='--', linewidth=2)
ax2.set_ylabel('Frequency', fontsize=13)

axes[1].legend(loc='upper left')
ax2.legend(loc='upper right')

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



Conclusions

Posterior Results:

- **Ω_m = 0.329 ± 0.017** (matter density)
- **h = 0.735 ± 0.002** (reduced Hubble constant)
- Strong anti-correlation: ρ(Ω_m, h) = -0.80

Cosmological Interpretation:

The matter density we found is **1σ higher** than Planck CMB (Ω_m = 0.315 ± 0.007), while the Hubble constant lies between Planck (h = 0.674) and SH0ES local measurements (h = 0.73). Inline with the ongoing hubble tension

HMC Performance:

The sampler achieved:

- **Convergence:** Geweke Z-scores < 2, stable trace plots
- **Efficiency:** N_eff = 256
- **Sensitivity to tuning:** ε = 2e-3, L = 50 is the only viable configuration in my testing, other choices lead to failures in the model.

Conclusion: The results confirm the accelerating expansion of the Universe measured with ~0.2% precision on h.

1.4. Optional Extension

- Write and apply a Gelman-Rubin convergence test, and deduce roughly how long the chains should be for convergence.

In [ ]:
```
# Optional: Gelman-Rubin convergence test
# Run multiple chains from different starting points
# Compute R-hat statistic
# Your code here
```