

# 期末專題：雙變量函數的繪圖 & 多變量函數的參數估計與極值計算

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作品目標：本作品分為兩部分

1. 混合常態參數估計 Normal Mixture
2. 限制式條件的最大值問題 Constraint optimization

藉由解決混合常態的參數估計以及限制式條件的最大值問題來練熟悉mle以及最佳化的概念

## 混合常態參數估計 Normal Mixture

### 單個圖形的繪製

```
In [ ]: from scipy.stats import beta, norm
import matplotlib.pyplot as plt
import numpy as np

# 樣本大小
n = 100000

# 兩個常態分配的參數
mu1, mu2 = 1, 9
sigma1, sigma2 = 2, 3

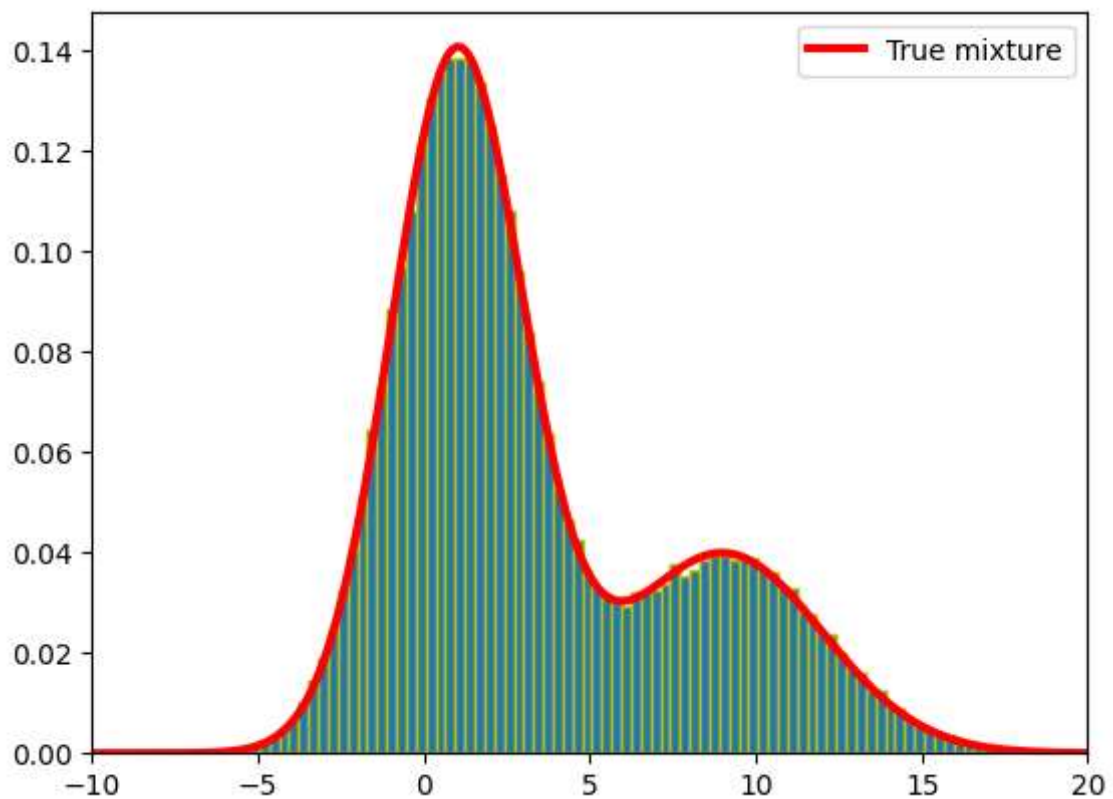
# 兩個常態分配的混合比例
p1 = 0.7

x = np.linspace(-50, 50, n)

# 混合常態分配的機率密度函數
y = p1 * norm.pdf(x, mu1, sigma1) + (1-p1) * norm.pdf(x, mu2, sigma2)
plt.plot(x, y, color='r', linewidth=3, label='True mixture')

n1 = int(n * p1)
n2 = n - n1
sample = np.r_[norm.rvs(mu1, sigma1, size=n1), norm.rvs(mu2, sigma2, size=n2)]

plt.hist(sample, bins=100, edgecolor='y', density=True)
plt.legend()
plt.xlim(-10, 20)
plt.show()
```



繪製多個圖形以供觀察

```
In [ ]: from scipy.stats import norm
import matplotlib.pyplot as plt
import numpy as np

# 樣本大小
n = 100000

# 兩個常態分佈的參數
mu1 = [1, 0, 1, 0, 0, 0]
sigma1 = [2, 1, 1, 1, 1, 1]
mu2 = [9, 3, 5, 2, 9, 9]
sigma2 = [3, 1, 4, 2, 1, 1]

# 混合常態分佈的比例
p1 = [0.5, 0.25, 0.8, 0.6, 0.5, 0.9]

x = np.linspace(-50, 50, n)

fig, ax = plt.subplots(2, 3, figsize=(30, 20))

def find_mix_pdf(x, mu1, sigma1, mu2, sigma2, p1):
    return p1 * norm.pdf(x, mu1, sigma1) + (1 - p1) * norm.pdf(x, mu2, sigma2)

for i in range(len(mu1)):

    # 計算混合常態分佈的機率密度函數
    y = find_mix_pdf(x, mu1[i], sigma1[i], mu2[i], sigma2[i], p1[i])

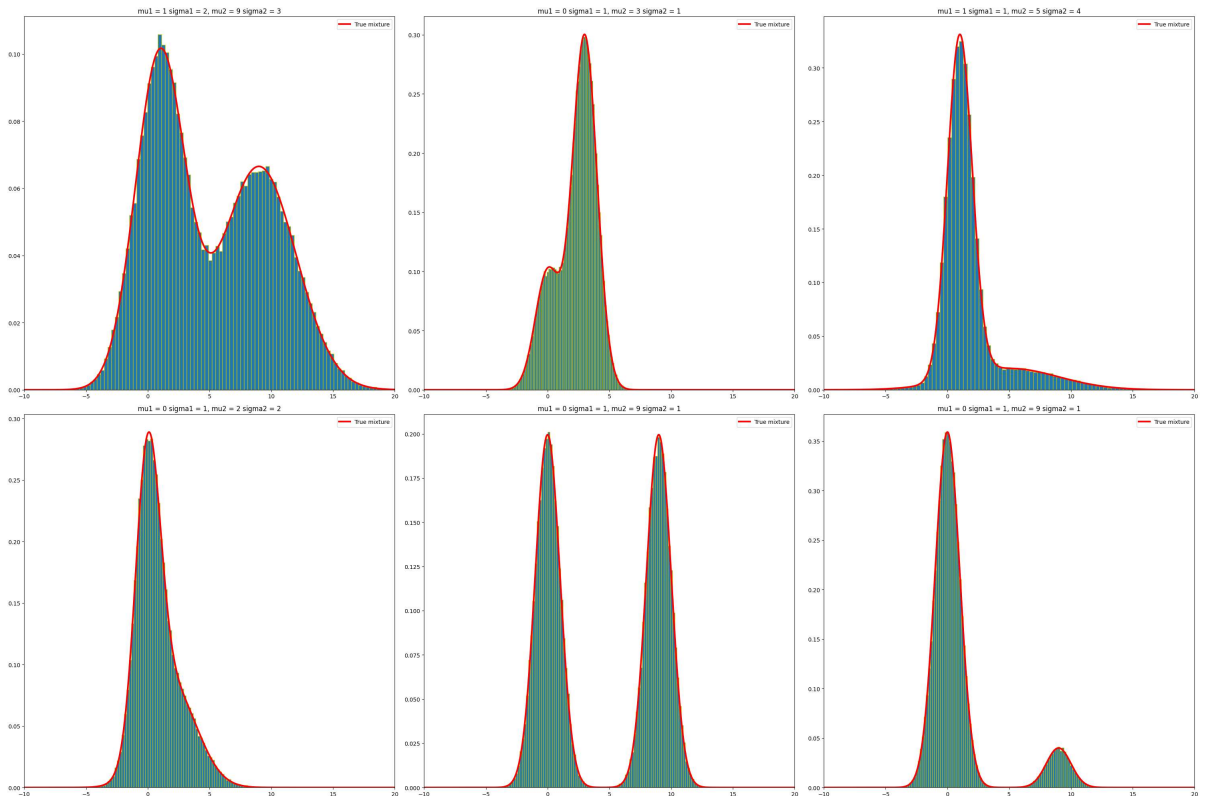
    # 計算混合常態分佈的樣本數量
    n1 = int(n * p1[i])
    n2 = n - n1
```

```
# 產生混合常態分佈的樣本
sample = np.concatenate([norm.rvs(mu1[i], sigma1[i], size=n1), norm.rvs(mu2[i],

ax[i // 3, i % 3].plot(x, y, color='r', linewidth=3, label='True mixture')
ax[i // 3, i % 3].hist(sample, bins=100, edgecolor='y', density=True)
ax[i // 3, i % 3].set_title("mu1 = {} sigma1 = {}, mu2 = {} sigma2 = {}".format
ax[i // 3, i % 3].legend()

# 把範圍限制在 -10 ~ 20 方便觀察
ax[i // 3, i % 3].set_xlim(-10, 20)

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



這六張圖由左至右、右上到下方分別為：

1. 平均數1、標準差2的常態與平均數9、標準差3的常態依據權重0.5混合而成
2. 平均數0、標準差1的常態與平均數3、標準差1的常態依據權重0.25混合而成
3. 平均數1、標準差1的常態與平均數5、標準差4的常態依據權重0.8混合而成
4. 平均數0、標準差1的常態與平均數2、標準差2的常態依據權重0.6混合而成
5. 平均數0、標準差1的常態與平均數9、標準差1的常態依據權重0.5混合而成
6. 平均數0、標準差1的常態與平均數9、標準差1的常態依據權重0.9混合而成

由這幾張圖可以看出以下幾點

1. 當兩個常態的平均越接近，混合的圖形的高峰會越平坦
2. 標準差越大，越容易有長尾的情況
3. 權重越大，出來的圖形會越往該常態的方向偏移

查看樣本數對於混合常態的影響

1. 根據mle函數，我們可以得到混合常態的參數估計值
2. 查看樣本數對於參數估計值的影響

```
In [ ]: import numpy as np
from scipy.stats import norm, binom
import matplotlib.pyplot as plt
import scipy.optimize as opt

def plot_mixture(pi1, mu1_list, sigma1_list, mu2_list, sigma2_list, n):
    num_plots = len(mu1_list)

    fig, ax = plt.subplots(2, 3, figsize=(30, 20))

    for i in range(num_plots):
        mu1 = mu1_list[i]
        sigma1 = sigma1_list[i]
        mu2 = mu2_list[i]
        sigma2 = sigma2_list[i]

        # 計算混合常態分佈的機率密度函數
        f = lambda x: pi1 * norm.pdf(x, mu1, sigma1) + (1 - pi1) * norm.pdf(x, mu2, sigma2)
        x = np.linspace(-50, 50, 10000)

        ax[i // 3, i % 3].plot(x, f(x), color='r', linewidth=3, label='True mixture')

        n1 = binom.rvs(n[i], pi1)
        n2 = n[i] - n1
        sample = np.concatenate([norm.rvs(mu1, sigma1, size=n1), norm.rvs(mu2, sigma2, size=n2)])

        ax[i // 3, i % 3].hist(sample, 50, edgecolor='y', density=True)

        # 透過最大概似法估計混合常態分佈的參數
        L = lambda x: -np.sum(np.log(x[0] * norm.pdf(sample, x[1], x[2]) + (1 - x[0]) * norm.pdf(sample, x[3], x[4])))

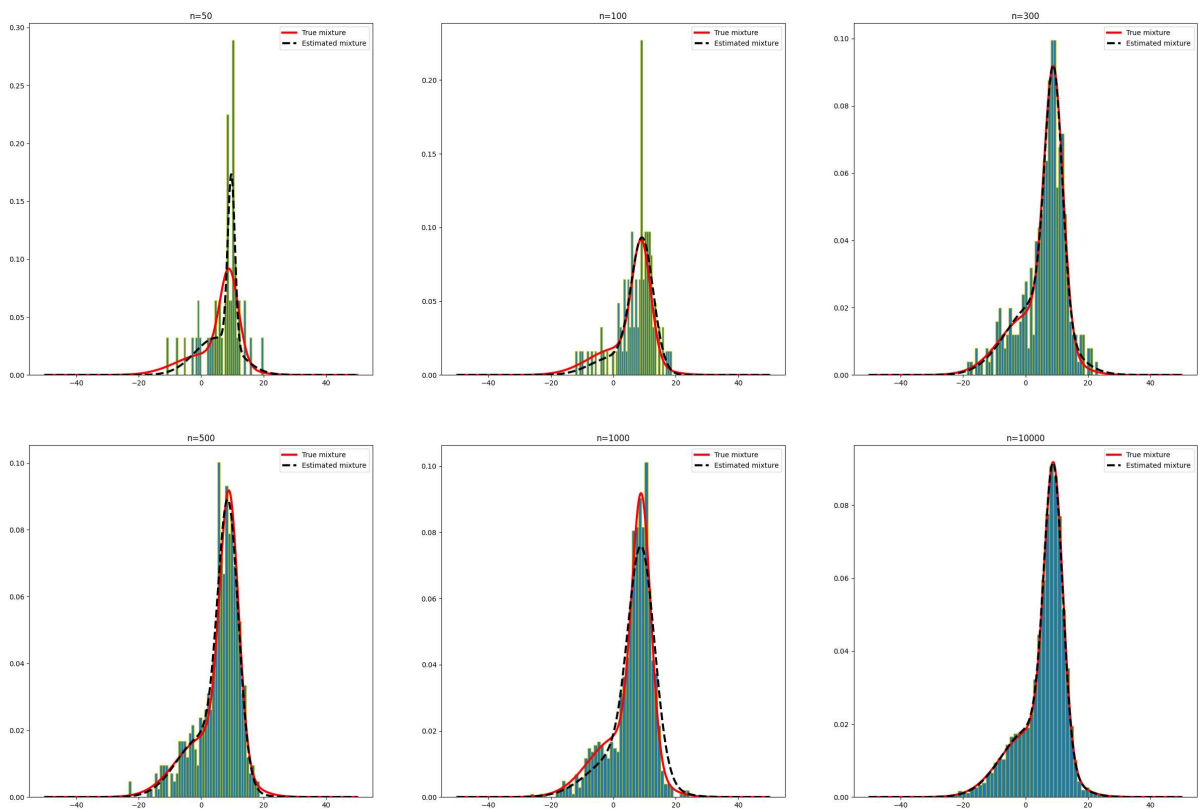
        bnds = [(0, 1), (0, np.inf), (0, np.inf), (0, np.inf), (0, np.inf)]
        opts = dict(dispatch = True, maxiter = 1e4)
        x0 = [0.5, 1, 10, 5, 5]

        res = opt.minimize(L, x0=x0, bounds=bnds, options=opts, tol=1e-8)

        f_hat = lambda x: res.x[0] * norm.pdf(x, res.x[1], res.x[2]) + (1 - res.x[0]) * norm.pdf(x, res.x[3], res.x[4])
        ax[i // 3, i % 3].plot(x, f_hat(x), color='k', linestyle='--', linewidth=3, label='MLE estimate')
        ax[i // 3, i % 3].set_title('n={}'.format(n[i]))
        ax[i // 3, i % 3].legend()

    plt.show()

pi1 = 0.4
mu1_list = [1,1,1,1,1,1]
sigma1_list = [9,9,9,9,9,9]
mu2_list = [9,9,9,9,9,9]
sigma2_list = [3,3,3,3,3,3]
n = [50,100,300,500,1000,10000]
plot_mixture(pi1, mu1_list, sigma1_list, mu2_list, sigma2_list, n)
```



上面的圖是以平均為1標準差為9的常態混合平均為9標準差為3的混合常態在樣本數為50,100,300,500,1000,10000時的實際值與估計值，由此張圖可以看出

1. 樣本數越大，估計值越接近實際值

## 使用GaussianMixture估計混合常態的參數

1. 使用GaussianMixture函數估計混合常態的參數，並與mle函數的結果做比較

```
In [ ]: import numpy as np
from scipy.stats import norm, binom
import matplotlib.pyplot as plt
import scipy.optimize as opt
from sklearn.mixture import GaussianMixture

def plot_mixture(pi1, mu1_list, sigma1_list, mu2_list, sigma2_list, n):
    num_plots = len(mu1_list)

    fig, ax = plt.subplots(2, 3, figsize=(30, 20))

    for i in range(num_plots):
        mu1 = mu1_list[i]
        sigma1 = sigma1_list[i]
        mu2 = mu2_list[i]
        sigma2 = sigma2_list[i]

        # 計算混合常態分佈的機率密度函數
        f = lambda x: pi1 * norm.pdf(x, mu1, sigma1) + (1 - pi1) * norm.pdf(x, mu2, sigma2)
        x = np.linspace(-50, 50, 10000)

        ax[i // 3, i % 3].plot(x, f(x), color='r', linewidth=3, label='True mixture')

        n1 = binom.rvs(n[i], pi1)
```

```

n2 = n[i] - n1
sample = np.concatenate([norm.rvs(mu1, sigma1, size=n1), norm.rvs(mu2, sigma2, size=n2)])

ax[i // 3, i % 3].hist(sample, 50, edgecolor='y', density=True)

# 透過最大概似法估計混合常態分佈的參數
L = lambda x: -np.sum(np.log(x[0] * norm.pdf(sample, x[1], x[2]) + (1 - x[0]) * norm.pdf(sample, x[3], x[4])))

bnds = [(0, 1), (0, np.inf), (0, np.inf), (0, np.inf), (0, np.inf)]
opts = dict(dispatch=True, maxiter=1e4)
x0 = [0.5, 1, 10, 5, 5]

res = opt.minimize(L, x0=x0, bounds=bnds, options=opts, tol=1e-8)

f_hat = lambda x: res.x[0] * norm.pdf(x, res.x[1], res.x[2]) + (1 - res.x[0]) * norm.pdf(x, res.x[3], res.x[4])
ax[i // 3, i % 3].plot(x, f_hat(x), color='k', linestyle='--', linewidth=3)

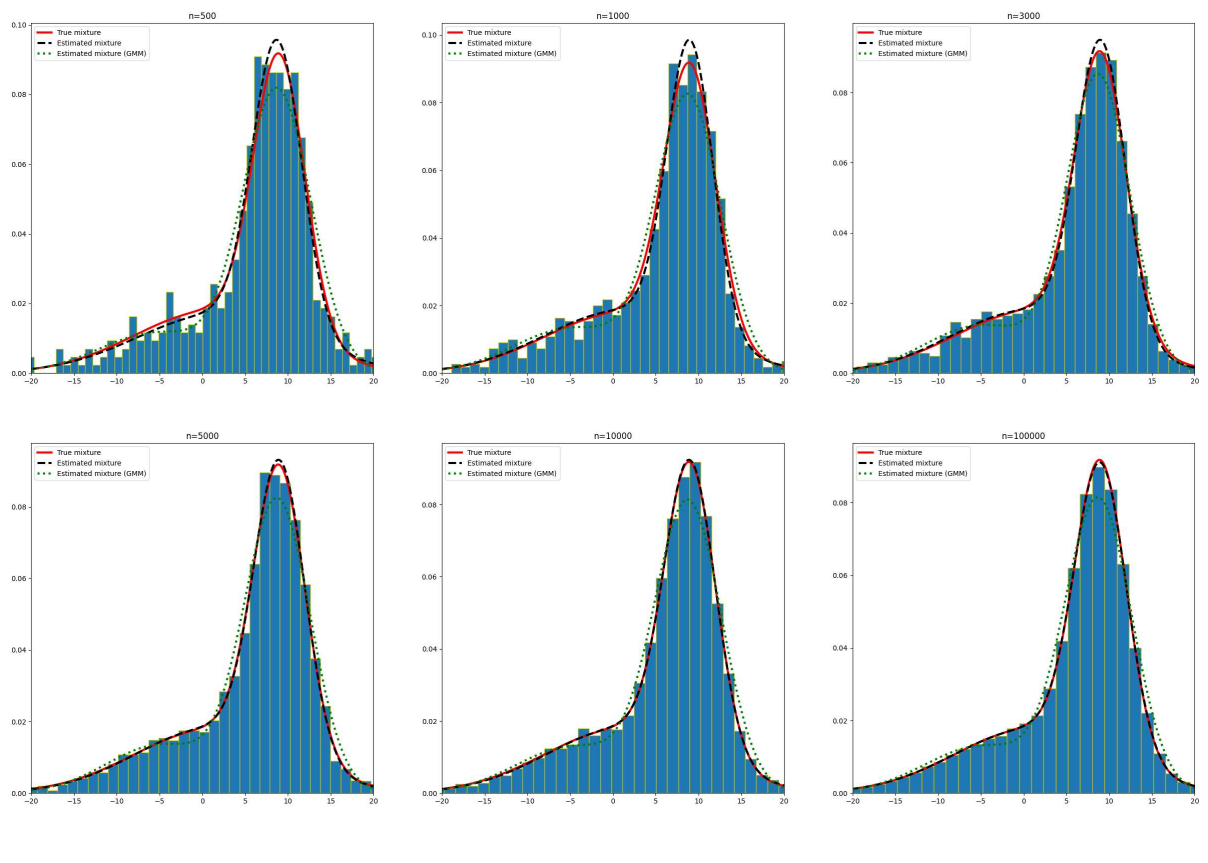
gmm = GaussianMixture(n_components=2, covariance_type='full')
gmm.fit(np.expand_dims(sample, 1))
gmm_density = np.exp(gmm.score_samples(np.expand_dims(x, 1)))
ax[i // 3, i % 3].plot(x, gmm_density, color='g', linestyle=':', linewidth=3)

ax[i // 3, i % 3].set_title('n={}'.format(n[i]))
ax[i // 3, i % 3].legend()
ax[i // 3, i % 3].set_xlim(-20, 20)

plt.show()

# Example usage with lists of parameters
pi1 = 0.4
mu1_list = [1,1,1,1,1,1]
sigma1_list = [9,9,9,9,9,9]
mu2_list = [9,9,9,9,9,9]
sigma2_list = [3,3,3,3,3,3]
n = [500,1000,3000,5000,10000,100000]
plot_mixture(pi1, mu1_list, sigma1_list, mu2_list, sigma2_list, n)

```



## 限制式條件的最大值問題 Constraint optimization

計算下列最大概似估計 MLE 問題的參數  $\alpha, \beta$  :

$$\max_{\alpha, \beta > 0} \ln L(\alpha, \beta)$$

其中的聯合概似函數為

$$L(\alpha, \beta) = \prod_{i=1}^n f_t(v_i | \alpha, \beta) F_T(u_i | \alpha, \beta)^{-1}$$

$$\text{where } f_t(v | \alpha, \beta) = \alpha \beta v^{\beta-1} \exp(-\alpha v^\beta)$$

$$F_T(u | \alpha, \beta) = 1 - \exp(-\alpha u^\beta)$$

以此函數作為聯合概似函數的目標函數

```
In [ ]: import numpy as np
import scipy.optimize as opt
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D

# 數據加載
data = np.loadtxt('uv.txt', skiprows=1)

U = data[:, 0]
V = data[:, 1]

# 目標函數定義(上面所推導的)
def log_likelihood(params):
    alpha, beta = params
    epsilon = 1e-10 # 小的偏移量以避免除零錯誤
    f_t = alpha * beta * V ** (beta - 1) * np.exp(-alpha * V ** beta) # 實現了 f_t
```



```

F_T = 1 - np.exp(-alpha * U ** beta) # 實現了  $F_T(u|\alpha, \beta) = 1 - \exp(-\alpha u^\beta)$ 
# 計算對數似然函數
return -np.sum(np.log(f_t / F_T + epsilon))

# 繪製目標函數的立體圖和等高線圖
alpha_range = np.linspace(0.1, 10, 100)
beta_range = np.linspace(0.1, 10, 100)
alpha_range = alpha_range[alpha_range != 0]
beta_range = beta_range[beta_range != 0]

Alpha, Beta = np.meshgrid(alpha_range, beta_range)
Z = np.array([log_likelihood([a, b]) for a, b in zip(np.ravel(Alpha), np.ravel(Beta))])
Z = Z.reshape(Alpha.shape)

# 立體圖
fig = plt.figure(figsize=(18, 8))
ax = fig.add_subplot(121, projection='3d')
ax.plot_surface(Alpha, Beta, Z, cmap='viridis')
ax.set_xlabel('Alpha')
ax.set_ylabel('Beta')
ax.set_zlabel('Log Likelihood')

# 等高線圖
ax2 = fig.add_subplot(122)
contour = ax2.contour(Alpha, Beta, Z, 50, cmap='viridis')
ax2.set_xlabel('Alpha')
ax2.set_ylabel('Beta')
# 使用之前定義的 log_likelihood 函數進行優化以找到極值
initial_params = [1, 1] # 初始猜測值
result = opt.minimize(log_likelihood, initial_params, method='L-BFGS-B', bounds=[(0.1, 10), (0.1, 10)])

# 獲得最佳參數
optimal_params = result.x
ax2.scatter(optimal_params[0], optimal_params[1], c='r', marker='x', s=100)
print('Optimal parameters are: {}'.format(optimal_params))
plt.title('Log Likelihood Contour')
plt.colorbar(contour, ax=ax2)

plt.show()

```

Optimal parameters are: [1.90735008 0.94643891]

