

1. Rosenbrock 函数（香蕉函数）

我们要采样的后验分布满足

$$\begin{aligned} \rho_{\text{post}}(\theta) &= e^{-\Phi_R(\theta)} \\ \Phi_R &= \frac{1}{2} \left((y - \mathcal{G}(\theta))^T \Sigma_{\eta}^{-1} (y - \mathcal{G}(\theta)) + (\theta - r_0)^T \Sigma_0^{-1} (\theta - r_0) \right) \\ &= \frac{1}{2} \left(\frac{100(\theta_2 - c_1\theta_1^2)^2}{c_2} + \frac{(1 - \theta_1)^2}{c_2} + \frac{\theta_1^2}{100} + \frac{\theta_2^2}{100} \right) \end{aligned}$$

暴力网格搜索

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In [3]: using PyPlot

function Phi_R_Rosenbrock(theta, theta, c1, c2)
    return (100*(theta2 - c1*theta1^2)^2/c2 + (1.0 - theta1)^2/c2 + theta1^2/100 + theta2^2/100)/2.0
end

Lx, Ux = -4.0, 8.0
Ly, Uy = -2.0, 10#3.5
N = 1000
X = zeros(N, N)
Y = zeros(N, N)
rho = zeros(N, N)
for i = 1:N
    for j = 1:N
        X[i, j], Y[i, j] = Lx + (Ux - Lx) * (i-1)/(N-1), Ly + (Uy - Ly) * (j-1)/(N-1)
    end
end
dx = dy = 1/(N-1)

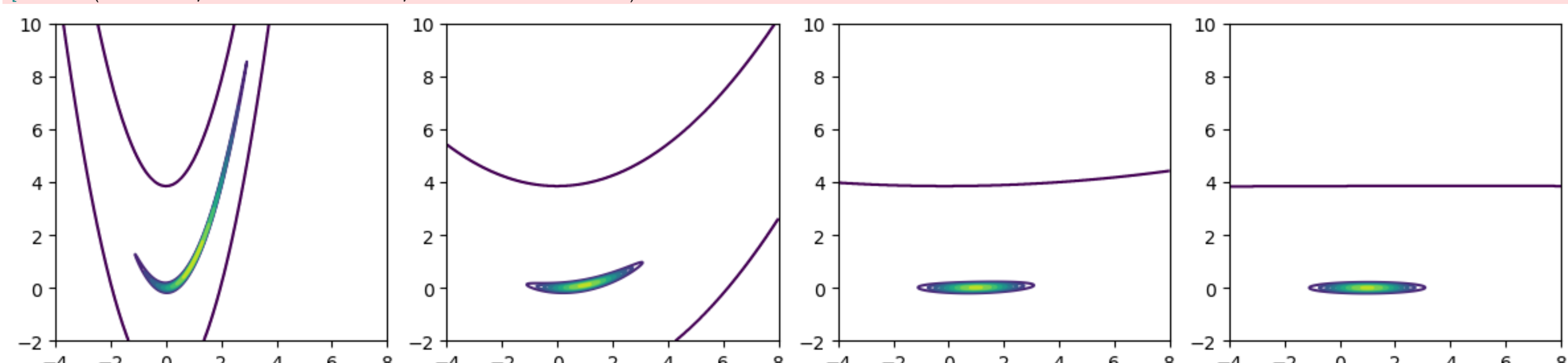
fig, ax = PyPlot.subplots(ncols=4, nrows=1, sharex=false, sharey=false, figsize=(12,3))

for k = 1:4
    c1, c2 = 10^(-(k-1.0)), 1.0
    for i = 1:N
        for j = 1:N
            rho[i, j] = Phi_R_Rosenbrock(X[i, j], Y[i, j], c1, c2)
        end
    end

    rho ./= exp.(-rho)
    Z = sum(rho)
    rho ./= Z
    rho ./= (dx * dy)
    ax[k].contour(X, Y, rho, 10)
    @info "mean = ", sum(X.*rho)/sum(rho), sum(Y.*rho)/sum(rho)
end

fig.tight_layout()
fig.savefig("Rosenbrock_1.pdf")
```

```
[ Info: ("mean = ", 0.9083223721468913, 1.686437532612661)
[ Info: ("mean = ", 0.9893276577929085, 0.19675099271002844)
[ Info: ("mean = ", 0.9900925963862894, 0.019701671046172844)
[ Info: ("mean = ", 0.9901002636870367, 0.001970193755655862)
```

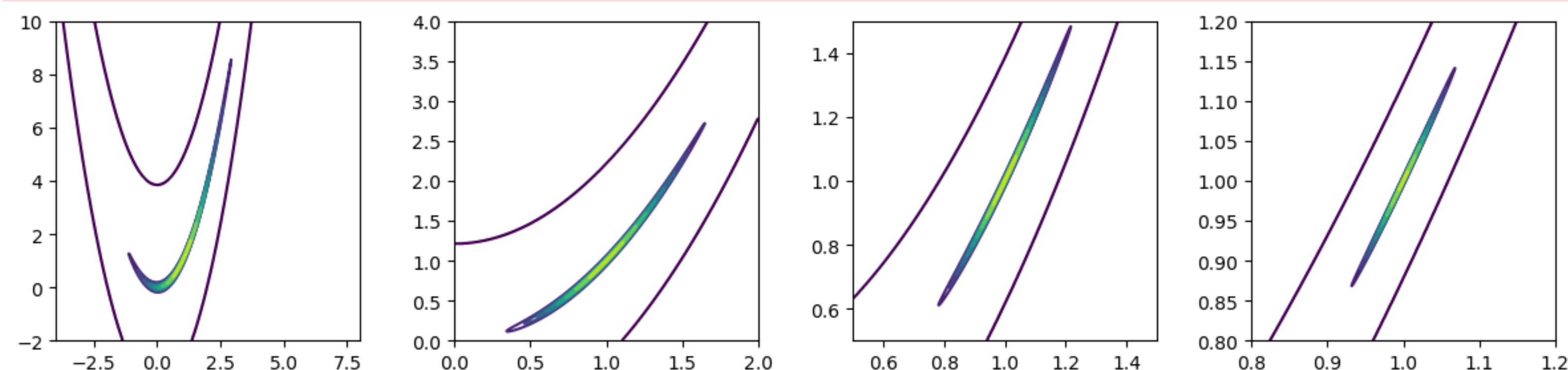


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In [4]: Lx, Ux = [-4.0;0.0;0.5;0.8], [8.0;2.0;1.5;1.2]
Ly, Uy = [-2.0;0.0;0.5;0.8], [10.0;4.0;1.5;1.2]
N = 1000
X = zeros(N, N)
Y = zeros(N, N)
rho = zeros(N, N)
for i = 1:N
    for j = 1:N
        X[i, j], Y[i, j] = Lx[k] + (Ux[k] - Lx[k]) * (i-1)/(N-1), Ly[k] + (Uy[k] - Ly[k]) * (j-1)/(N-1)
        rho[i, j] = Phi_R_Rosenbrock(X[i, j], Y[i, j], c1, c2)
    end
end

rho ./= exp.(-rho)
Z = sum(rho)
rho ./= Z
rho ./= (dx * dy)
ax[k].contour(X, Y, rho, 10)
@info "mean = ", sum(X.*rho)/sum(rho), sum(Y.*rho)/sum(rho)
end

fig.tight_layout()
fig.savefig("Rosenbrock_2.pdf")
```

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[ Info: ("mean = ", 0.9083223721468913, 1.686437532612661)
[ Info: ("mean = ", 0.9978348801870758, 1.092302714586285)
[ Info: ("mean = ", 0.997052605773829, 1.0032053198267843)
[ Info: ("mean = ", 0.9998858462934318, 1.0007534734013894)
```



2. Bernstein Von Mises 理论

对于后验分布，我们有

$$\begin{aligned} \rho_{\text{post}}(\theta) &= e^{-\Phi_R(\theta)} \quad \Phi_R = \frac{1}{2} \left(\frac{1}{\gamma^2} \Phi(\theta) + R(\theta) \right) \\ \Phi(\theta) &= (y - \mathcal{G}(\theta))^T \Sigma_{\eta}^{-1} (y - \mathcal{G}(\theta)) \quad R(\theta) = (\theta - r_0)^T \Sigma_0^{-1} (\theta - r_0) \end{aligned}$$

假设 $\Phi(\theta)$ 的极小值是 θ^{\dagger} ，那么当 $\gamma \rightarrow 0$

$$\frac{\rho_{\text{post}}(\theta^{\dagger})}{\rho_{\text{post}}(\theta)} = e^{\frac{1}{2}(\Phi(\theta) - \Phi(\theta^{\dagger})) + R(\theta) - R(\theta^{\dagger})} \rightarrow 0$$

质量将集中在 θ^{\dagger} 附近，我们可以线性化，转化为线性贝叶斯问题处理。

数据足够多，也可以转化成误差足够小。

2. 多峰函数

我们要采样的后验分布满足

$$\begin{aligned} \rho_{\text{post}}(\theta) &= e^{-\Phi_R(\theta)} \\ \Phi_R &= \frac{1}{2} \left((y - \mathcal{G}(\theta))^T \Sigma_{\eta}^{-1} (y - \mathcal{G}(\theta)) + (\theta - r_0)^T \Sigma_0^{-1} (\theta - r_0) \right) \\ &= \frac{1}{2} \left((4 - (\theta_2 - \theta_1)^2)^2 + (c - \theta_1)^2 + \theta_2^2 \right) \end{aligned}$$

```
In [5]: using PyPlot

using PyPlot

function Phi_R_Multimodal(theta, theta, c)
    return ((4 - (theta2 - theta1)^2)^2 + (theta1 - c)^2 + theta2^2)/2.0
end

Lx, Ux = -3.0, 3.0
Ly, Uy = -3.0, 3.0
N = 1000
X = zeros(N, N)
Y = zeros(N, N)
rho = zeros(N, N)
for i = 1:N
    for j = 1:N
        X[i, j], Y[i, j] = Lx + (Ux - Lx) * (i-1)/(N-1), Ly + (Uy - Ly) * (j-1)/(N-1)
    end
end

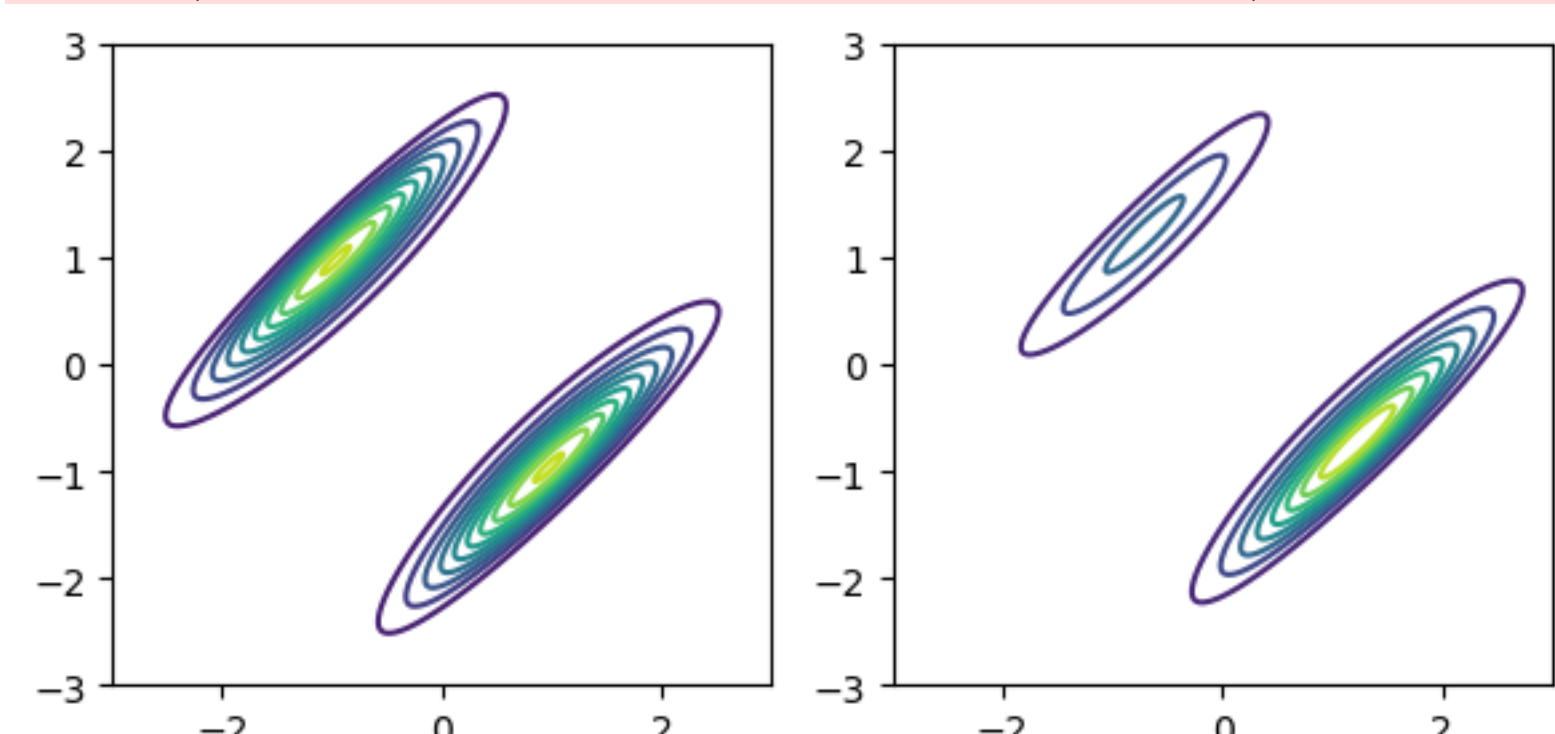
fig, ax = PyPlot.subplots(ncols=2, nrows=1, sharex=false, sharey=false, figsize=(6,3))

for k = 1:2
    c = 0.5*(k-1)
    for i = 1:N
        for j = 1:N
            rho[i, j] = Phi_R_Multimodal(X[i, j], Y[i, j], c)
        end
    end

    rho ./= exp.(-rho)
    Z = sum(rho)
    rho ./= Z
    rho ./= (dx * dy)
    ax[k].contour(X, Y, rho, 10)
    @info "mean = ", sum(X.*rho)/sum(rho), sum(Y.*rho)/sum(rho)
end

fig.tight_layout()
fig.savefig("Multimodal.pdf")
```

```
[ Info: ("mean = ", 0.0, 0.0)
[ Info: ("mean = ", 0.659067998901734, -0.17944598027399047)
```



In []: