

题干

- 考虑如下概率图模型(图略):
 - 写出对应的因子图
 - 使用和积算法 (sum-product algorithm) 计算边缘概率 $p(x_2)$
- 详细推导高斯混合模型 (Gaussian mixture model) 的 **E 步** 与 **M 步**
- 使用平均场方法 (mean field method) 近似高斯混合模型的边缘概率 $p_\theta(X)$ 。
变分分布为乘积形式:

$$q(Z, \pi, \mu_k, \Sigma_k) = q(Z)q(\pi) \prod_{k=1}^K q(\mu_k, \Sigma_k)$$

- 编写一个简单的 **拒绝采样 (rejection sampling)** Python 代码
- 考虑一个转移矩阵为

$$P = \begin{bmatrix} p_{11} & p_{12} & p_{13} \\ p_{21} & p_{22} & p_{23} \\ p_{31} & p_{32} & p_{33} \end{bmatrix}$$

的马尔可夫链。设 $\pi = (\pi_1, \pi_2, \pi_3)$ 是平稳分布, 求 π 应满足的方程。

- 为以下 MCMC 方法编写 Python 代码:
 - 基本 MCMC
 - 哈密顿蒙特卡洛 (Hamiltonian MC)
 - 朗之万动力学 (Langevin dynamics)
 用你的代码对一般的二维高斯分布进行采样, 比较三种方法的结果 (如接受率等)。
- 证明: **吉布斯采样 (Gibbs sampling)** 满足细致平衡条件 (detailed balance condition)。

Solution of T1

因子图

$$p(Z_1, Z_2, Z_3, X_1, X_2, X_3) = p(Z_1)p(Z_2 | Z_1)p(Z_3 | Z_2)p(X_1 | Z_1)p(X_2 | Z_2)p(X_3 | Z_3).$$

所以我们有 6 个因子 (把每个括号内的项作为一个因子):

$$f_{Z1} = p(Z_1), f_{Z2} = p(Z_2 | Z_1), f_{Z3} = p(Z_3 | Z_2), f_{X1} = p(X_1 | Z_1), f_{X2} = p(X_2 | Z_2), f_{X3} = p(X_3 | Z_3).$$

因子图如下 (小括号代表圆圈, 中括号代表正方形):

$$\begin{array}{ccccc} [f_{Z1}] & - & (Z1) & - & [f_{Z2}] & - & (Z2) & - & [f_{Z3}] & - & (Z3) \\ | & & & & | & & & & | & & \\ [f_{X1}] & & & & [f_{X2}] & & & & [f_{X3}] & & \\ | & & & & | & & & & | & & \\ (X1) & & & & (X2) & & & & (X3) & & \end{array}$$

边际概率

叶节点的传播:

$$\begin{aligned} \mu_{X1 \rightarrow f_{X1}}(x_1) &= 1, & \mu_{X3 \rightarrow f_{X3}}(x_3) &= 1. \\ \mu_{f_{X1} \rightarrow Z1}(z_1) &= \sum_{x_1} p(x_1 | z_1) = 1, & \mu_{f_{X3} \rightarrow Z3}(z_3) &= \sum_{x_3} p(x_3 | z_3) = 1. \end{aligned}$$

从左侧传来的部分:

$$\begin{aligned} \mu_{f_{Z1} \rightarrow Z1}(z_1) &= p(z_1). \\ \mu_{Z1 \rightarrow f_{Z2}}(z_1) &= p(z_1) \cdot 1 = p(z_1). \end{aligned}$$

$$\mu_{f_{Z_2 \rightarrow Z_2}}(z_2) = \sum_{z_1} p(z_2|z_1)p(z_1) = p(z_2).$$

从右侧传来的部分:

$$\mu_{Z_3 \rightarrow f_{Z_3}}(z_3) = 1.$$

$$\mu_{f_{Z_3 \rightarrow Z_2}}(z_2) = \sum_{z_3} p(z_3|z_2) = 1.$$

Z_2 的总消息:

$$\mu_{Z_2 \rightarrow f_{X_2}}(z_2) = \mu_{f_{Z_2 \rightarrow Z_2}}(z_2) \cdot \mu_{f_{Z_3 \rightarrow Z_2}}(z_2) = p(z_2) \cdot 1 = p(z_2).$$

从而 X_2 的边缘概率:

$$p(x_2) = \mu_{f_{X_2 \rightarrow X_2}}(x_2) = \sum_{z_2} p(x_2|z_2)p(z_2).$$

其中

$$p(z_2) = \sum_{z_1} p(z_1)p(z_2|z_1).$$

即:

$$p(x_2) = \sum_{z_2} p(x_2 | z_2) \left(\sum_{z_1} p(z_1) p(z_2 | z_1) \right)$$

Solution of T2

回忆GMM模型的设定：假设我们有N个观测数据 x_1, x_2, \dots, x_N ，假设它们独立同分布，服从K个高斯分布的混合：

$$p(x_n | \Theta) = \sum_{k=1}^K \pi_k \mathcal{N}(x_n | \mu_k, \Sigma_k)$$

其中：

- π_k 是混合权重，满足 $\sum_k \pi_k = 1$ 且 $\pi_k \geq 0$
- μ_k 和 Σ_k 分别是第k个高斯的均值和协方差矩阵
- $\Theta = \{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$ 是所有参数

隐变量 z_n 表示第n个样本属于哪一类：

$$z_n = [z_{n1}, z_{n2}, \dots, z_{nK}], \quad z_{nk} \in 0, 1, \quad \sum_k z_{nk} = 1$$

则complete-data likelihood为：

$$p(\{x_n, z_n\}_{n=1}^N | \Theta) = \prod_{n=1}^N \prod_{k=1}^K [\pi_k \mathcal{N}(x_n | \mu_k, \Sigma_k)]^{z_{nk}}$$

对数似然：

$$\ln p(X, Z | \Theta) = \sum_{n=1}^N \sum_{k=1}^K z_{nk} \left[\ln \pi_k + \ln \mathcal{N}(x_n | \mu_k, \Sigma_k) \right]$$

E-Step

在E-step，我们希望计算隐变量的后验期望

$$\gamma_{nk} \equiv \mathbb{E}[z_{nk} | x_n, \Theta^{\text{old}}] = p(z_{nk} = 1 | x_n, \Theta^{\text{old}})$$

根据贝叶斯公式：

$$\gamma_{nk} = p(z_{nk} = 1 \mid x_n, \Theta^{\text{old}}) = \frac{\pi_k \mathcal{N}(x_n \mid \mu_k, \Sigma_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(x_n \mid \mu_j, \Sigma_j)}$$

M-Step

在M-step，我们希望最大化期望对数似然

定义Q 函数：

$$Q(\Theta, \Theta^{\text{old}}) = \mathbb{E}_{Z|X, \Theta^{\text{old}}}[\ln p(X, Z \mid \Theta)] = \sum_{n=1}^N \sum_{k=1}^K \gamma_{nk} \left[\ln \pi_k + \ln \mathcal{N}(x_n \mid \mu_k, \Sigma_k) \right]$$

以下分别对 π_k 、 μ_k 、 Σ_k 求最大化。

由于有约束条件 $\sum_k \pi_k = 1$ 。引入拉格朗日乘子：

$$\mathcal{L} = \sum_{n=1}^N \sum_{k=1}^K \gamma_{nk} \ln \pi_k + \lambda \left(\sum_{k=1}^K \pi_k - 1 \right)$$

Q 对 π_k 求导数为 0：

$$\frac{\partial \mathcal{L}}{\partial \pi_k} = \sum_{n=1}^N \frac{\gamma_{nk}}{\pi_k} + \lambda = 0 \quad \Rightarrow \quad \pi_k = -\frac{1}{\lambda} \sum_{n=1}^N \gamma_{nk}$$

利用约束 $\sum_k \pi_k = 1$ ：

$$\sum_k \pi_k = -\frac{1}{\lambda} \sum_k \sum_n \gamma_{nk} = -\frac{1}{\lambda} \sum_n \sum_k \gamma_{nk} = -\frac{1}{\lambda} N = 1 \quad \Rightarrow \quad \lambda = -N$$

所以更新公式：

$$\pi_k^{\text{new}} = \frac{1}{N} \sum_{n=1}^N \gamma_{nk}$$

因为：

$$\ln \mathcal{N}(x_n \mid \mu_k, \Sigma_k) = -\frac{1}{2} (x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k) + \text{const}$$

因此 Q 对 μ_k 求导并令导数为 0：

$$\sum_{n=1}^N \gamma_{nk} \Sigma_k^{-1} (x_n - \mu_k) = 0 \quad \Rightarrow \quad \mu_k^{\text{new}} = \frac{\sum_{n=1}^N \gamma_{nk} x_n}{\sum_{n=1}^N \gamma_{nk}}$$

Q 对 Σ_k 进行矩阵求导并令导数为 0：考虑到 Σ_k 是对称正定矩阵，使用矩阵求导公式 $\frac{\partial \ln |\Sigma|}{\partial \Sigma} = (\Sigma^{-1})^T = \Sigma^{-1}$ ， $\frac{\partial}{\partial \Sigma} [x^T \Sigma^{-1} x] = -\Sigma^{-1} x x^T \Sigma^{-1}$ ，因此求导结果如下：

$$\frac{\partial L}{\partial \Sigma_k} = -\frac{1}{2} \sum_{n=1}^N \gamma_{nk} [\Sigma_k^{-1} - \Sigma_k^{-1} (x_n - \mu_k)(x_n - \mu_k)^T \Sigma_k^{-1}] = 0$$

化简后解得：

$$\Sigma_k^{\text{new}} = \frac{\sum_{n=1}^N \gamma_{nk} (x_n - \mu_k^{\text{new}})(x_n - \mu_k^{\text{new}})^T}{\sum_{n=1}^N \gamma_{nk}}$$

综上所述：

E 步：

$$\gamma_{nk} = \frac{\pi_k \mathcal{N}(x_n \mid \mu_k, \Sigma_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(x_n \mid \mu_j, \Sigma_j)}$$

M 步：

$$\begin{aligned}\pi_k^{\text{new}} &= \frac{1}{N} \sum_{n=1}^N \gamma_{nk} \\ \mu_k^{\text{new}} &= \frac{\sum_{n=1}^N \gamma_{nk} x_n}{\sum_{n=1}^N \gamma_{nk}} \\ \Sigma_k^{\text{new}} &= \frac{\sum_{n=1}^N \gamma_{nk} (x_n - \mu_k^{\text{new}})(x_n - \mu_k^{\text{new}})^T}{\sum_{n=1}^N \gamma_{nk}}\end{aligned}$$

Solution of T3

整体想法是用ELBO近似 $\log p_\theta(X)$ ，于是 $p_\theta(X) \approx \exp\{ELBO\}$ 。

高斯混合模型的联合分布为：

$$p_\theta(X, Z, \pi, \mu, \Sigma) = p(Z|\pi)p(X|Z, \mu, \Sigma)p(\pi)p(\mu, \Sigma)$$

其中 Z 为离散隐变量， π 为混合权重， μ_k, Σ_k 为第k个高斯分量的参数。依题意，变分分布为：

$$q(Z, \pi, \mu_k, \Sigma_k) = q(Z)q(\pi) \prod_{k=1}^K q(\mu_k, \Sigma_k)$$

因此ELBO的表达式为：

$$\begin{aligned}\mathcal{L}(q) &= \mathbb{E}_q \left[\log \frac{p_\theta(X, Z, \pi, \mu, \Sigma)}{q(Z, \pi, \mu, \Sigma)} \right] \\ &= \mathbb{E}_q[\log p(X|Z, \mu, \Sigma)] + \mathbb{E}_q[\log p(Z|\pi)] + \mathbb{E}_q[\log p(\pi)] + \mathbb{E}_q[\log p(\mu, \Sigma)] \\ &\quad - \mathbb{E}_q[\log q(Z)] - \mathbb{E}_q[\log q(\pi)] - \sum_{k=1}^K \mathbb{E}_q[\log q(\mu_k, \Sigma_k)]\end{aligned}$$

以下用EM algorithm，固定其他变分因子，分别优化每个因子。先更新 $q(Z)$ ：

$$\log q^*(Z) = \mathbb{E}_{q(\pi)q(\mu, \Sigma)}[\log p(X, Z, \pi, \mu, \Sigma)] + \text{const}$$

$$q^*(Z) = \prod_{n=1}^N \prod_{k=1}^K r_{nk}^{z_{nk}}$$

其中：

$$r_{nk} \propto \exp \left(\mathbb{E}[\log \pi_k] - \frac{1}{2} \mathbb{E}[(\mathbf{x}_n - \mu_k)^T \Sigma_k^{-1} (\mathbf{x}_n - \mu_k)] - \frac{1}{2} \mathbb{E}[\log |\Sigma_k|] \right)$$

再更新 $q(\pi)$ ：

$$\log q^*(\pi) = \mathbb{E}_{q(Z)}[\log p(Z|\pi)] + \log p(\pi) + \text{const}$$

这里的先验通常取Dirichlet分布： $p(\pi) = \text{Dir}(\pi|\alpha)$ ，此时：

$$q^*(\pi) = \text{Dir}(\pi|\alpha^*), \quad \alpha_k^* = \alpha_k + \sum_{n=1}^N \mathbb{E}[z_{nk}]$$

再更新 $q(\mu_k, \Sigma_k)$ ：

$$\log q^*(\mu_k, \Sigma_k) = \mathbb{E}_{q(Z)}[\log p(X|Z, \mu_k, \Sigma_k)] + \log p(\mu_k, \Sigma_k) + \text{const}$$

这里的先验通常取高斯-逆Wishart先验，此时 $q(\mu_k, \Sigma_k)$ 也是高斯-逆Wishart分布。

重复直到收敛，最后用最终的 $\mathcal{L}(q)$ 近似 $\log p_\theta(X)$ ，即

$$p_\theta(X) \approx \exp(\mathcal{L}(q))$$

其中 $\mathcal{L}(q)$ 是收敛后的变分下界值。

Solution of T4

以下以生成(-5,5)上的服从 $f(x) = \frac{1}{\sqrt{2\pi}}e^{-x^2/2}$ 的随机变量为例, 代码如下:

```
import numpy as np

def simple_rejection_sampling():
    def complex_target(x):
        # 这里写出pdf的表达式
        return (1 / np.sqrt(2 * np.pi)) * np.exp(-x**2 / 2)

    n_samples = 1000
    samples = []

    # 确定M
    x_test = np.linspace(-5, 5, 1000)
    max_value = np.max(complex_target(x_test))
    M = max_value + 0.1

    while len(samples) < n_samples:
        x_proposal = np.random.uniform(-5, 5)
        u = np.random.uniform(0, 1)
        acceptance_prob = complex_target(x_proposal) / M

        if u < acceptance_prob:
            samples.append(x_proposal)

    return samples

# 生成随机样本
simple_samples = simple_rejection_sampling()
print(f"\n简单示例生成了 {len(simple_samples)} 个样本")
```

Solution of T5

由于 $\pi = (\pi_1, \pi_2, \pi_3)$ 是一个平稳分布, 因此:

$$\pi P = \pi \quad \pi_1 + \pi_2 + \pi_3 = 1, \quad \pi_i \geq 0$$

所以:

$$[\pi_1, \pi_2, \pi_3] \begin{bmatrix} p_{11} & p_{12} & p_{13} \\ p_{21} & p_{22} & p_{23} \\ p_{31} & p_{32} & p_{33} \end{bmatrix} = [\pi_1, \pi_2, \pi_3]$$

即:

$$\begin{bmatrix} p_{11} - 1 & p_{21} & p_{31} \\ p_{12} & p_{22} - 1 & p_{32} \\ p_{13} & p_{23} & p_{33} - 1 \end{bmatrix} \begin{bmatrix} \pi_1 \\ \pi_2 \\ \pi_3 \end{bmatrix} = 0 \quad \cdots \quad (*)$$

因为 P 是随机矩阵, 有:

$$\begin{aligned} p_{11} + p_{12} + p_{13} &= 1 \\ p_{21} + p_{22} + p_{23} &= 1 \\ p_{31} + p_{32} + p_{33} &= 1 \end{aligned}$$

故在(*)两端左乘如下矩阵:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 1 & 1 \end{bmatrix}$$

得到:

$$\begin{bmatrix} p_{11} - 1 & p_{21} & p_{31} \\ p_{12} & p_{22} - 1 & p_{32} \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \pi_1 \\ \pi_2 \\ \pi_3 \end{bmatrix} = 0$$

即满足两个方程, 再加上方程 $\pi_1 + \pi_2 + \pi_3 = 1$, 即可得到 π 满足的方程组:

$$\begin{bmatrix} p_{11} - 1 & p_{21} & p_{31} \\ p_{12} & p_{22} - 1 & p_{32} \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} \pi_1 \\ \pi_2 \\ \pi_3 \end{bmatrix} = 0$$

或者等价地写成:

$$\begin{cases} \pi_1(p_{11} - 1) + \pi_2 p_{21} + \pi_3 p_{31} = 0 \\ \pi_1 p_{12} + \pi_2(p_{22} - 1) + \pi_3 p_{32} = 0 \\ \pi_1 + \pi_2 + \pi_3 = 1 \end{cases}$$

Solution of T6

```
import numpy as np
from scipy.stats import multivariate_normal

class BasicMCMC:
    """Basic MCMC method (Metropolis-Hastings)"""

    def __init__(self, target_dist, proposal_std=1.0):
        self.target_dist = target_dist
        self.proposal_std = proposal_std

    def sample(self, n_samples, initial_state, burn_in=1000):
        current_state = initial_state
        samples = []
        accepted = 0

        for i in range(n_samples + burn_in):
            # Generate candidate sample (normal distribution proposal)
            proposal = current_state + np.random.normal(0, self.proposal_std, size=current_state.shape)

            # Calculate acceptance probability
            current_prob = self.target_dist(current_state)
            proposal_prob = self.target_dist(proposal)
            acceptance_ratio = min(1, proposal_prob / current_prob)

            # Accept or reject
            if np.random.rand() < acceptance_ratio:
                current_state = proposal
                if i >= burn_in:
                    accepted += 1

            if i >= burn_in:
                samples.append(current_state.copy())

        acceptance_rate = accepted / n_samples
        return np.array(samples), acceptance_rate

class HamiltonianMC:
    """Hamiltonian Monte Carlo method"""

    def __init__(self, target_dist, step_size=0.1, n_leapfrog=10, mass=1.0):
        self.target_dist = target_dist
        self.step_size = step_size
        self.n_leapfrog = n_leapfrog
        self.mass = mass

    def kinetic_energy(self, momentum):
        """Kinetic energy"""
        return 0.5 * np.sum(momentum**2) / self.mass

    def potential_energy(self, position):
        """Potential energy (negative log probability)"""
        return -np.log(self.target_dist(position) + 1e-10)

    def hamiltonian(self, position, momentum):
        """Hamiltonian"""
        return self.potential_energy(position) + self.kinetic_energy(momentum)

    def leapfrog_step(self, position, momentum):
        """Leapfrog integration step"""
        # Half step update momentum
        grad = self.numerical_gradient(position)
        momentum = momentum - 0.5 * self.step_size * grad
```

```

# Full step update position
position = position + self.step_size * momentum / self.mass

# Half step update momentum
grad = self.numerical_gradient(position)
momentum = momentum - 0.5 * self.step_size * grad

return position, momentum

def numerical_gradient(self, position, eps=1e-6):
    """Numerical gradient calculation"""
    grad = np.zeros_like(position)
    for i in range(len(position)):
        pos_plus = position.copy()
        pos_minus = position.copy()
        pos_plus[i] += eps
        pos_minus[i] -= eps
        grad[i] = (self.potential_energy(pos_plus) - self.potential_energy(pos_minus)) / (2 * eps)
    return grad

def sample(self, n_samples, initial_state, burn_in=1000):
    current_state = initial_state
    samples = []
    accepted = 0

    for i in range(n_samples + burn_in):
        # Sample momentum from normal distribution
        current_momentum = np.random.normal(0, np.sqrt(self.mass), size=current_state.shape)

        # Leapfrog integration to simulate trajectory
        proposed_state = current_state.copy()
        proposed_momentum = current_momentum.copy()

        for _ in range(self.n_leapfrog):
            proposed_state, proposed_momentum = self.leapfrog_step(proposed_state, proposed_momentum)

        # Calculate Hamiltonian
        current_hamiltonian = self.hamiltonian(current_state, current_momentum)
        proposed_hamiltonian = self.hamiltonian(proposed_state, -proposed_momentum) # Momentum reversal

        # Acceptance probability
        acceptance_ratio = min(1, np.exp(current_hamiltonian - proposed_hamiltonian))

        # Accept or reject
        if np.random.rand() < acceptance_ratio:
            current_state = proposed_state
            if i >= burn_in:
                accepted += 1

        if i >= burn_in:
            samples.append(current_state.copy())

    acceptance_rate = accepted / n_samples
    return np.array(samples), acceptance_rate

class LangevinDynamics:
    """Langevin Dynamics MCMC"""

    def __init__(self, target_dist, step_size=0.1, mass=1.0):
        self.target_dist = target_dist
        self.step_size = step_size
        self.mass = mass

```

```

def potential_energy(self, position):
    """Potential energy (negative log probability)"""
    return -np.log(self.target_dist(position) + 1e-10)

def numerical_gradient(self, position, eps=1e-6):
    """Numerical gradient calculation"""
    grad = np.zeros_like(position)
    for i in range(len(position)):
        pos_plus = position.copy()
        pos_minus = position.copy()
        pos_plus[i] += eps
        pos_minus[i] -= eps
        grad[i] = (self.potential_energy(pos_plus) - self.potential_energy(pos_minus)) / (2 * eps)
    return grad

def sample(self, n_samples, initial_state, burn_in=1000):
    current_state = initial_state
    samples = []

    for i in range(n_samples + burn_in):
        # Langevin dynamics update
        grad = self.numerical_gradient(current_state)
        noise = np.random.normal(0, np.sqrt(2 * self.step_size), size=current_state.shape)

        current_state = current_state - self.step_size * grad + noise

        if i >= burn_in:
            samples.append(current_state.copy())

    # Langevin dynamics typically has high acceptance rate (close to 1)
    acceptance_rate = 1.0 # Simplified estimation
    return np.array(samples), acceptance_rate

# Testing and comparison
def main():
    # Set up target distribution: 2D Gaussian
    mean = np.array([1.0, -1.0])
    cov = np.array([[2.0, 0.8], [0.8, 1.5]])
    target_dist = multivariate_normal(mean, cov)

    def target_pdf(x):
        return target_dist.pdf(x)

    # Parameter settings
    n_samples = 5000
    burn_in = 1000
    initial_state = np.array([0.0, 0.0])

    # Basic MCMC
    print("Running Basic MCMC...")
    basic_mcmc = BasicMCMC(target_pdf, proposal_std=1.0)
    samples_basic, acc_basic = basic_mcmc.sample(n_samples, initial_state, burn_in)

    # Hamiltonian Monte Carlo
    print("Running Hamiltonian Monte Carlo...")
    hmc = HamiltonianMC(target_pdf, step_size=0.1, n_leapfrog=10)
    samples_hmc, acc_hmc = hmc.sample(n_samples, initial_state, burn_in)

    # Langevin Dynamics
    print("Running Langevin Dynamics...")
    langevin = LangevinDynamics(target_pdf, step_size=0.01)
    samples_langevin, acc_langevin = langevin.sample(n_samples, initial_state, burn_in)

    # Print acceptance rate comparison

```

```

print("\n=== Acceptance Rate Comparison ===")
print(f"Basic MCMC: {acc_basic:.3f}")
print(f"HMC: {acc_hmc:.3f}")
print(f"Langevin Dynamics: {acc_langevin:.3f}")

if __name__ == "__main__":
    main()

```

运行结果如下:

```

=== Acceptance Rate Comparison ===
Basic MCMC: 0.606
HMC: 1.000
Langevin Dynamics: 1.000

```

Solution of T7

设 d 维随机变量 $\mathbf{x} = (x_1, \dots, x_d)$, 目标分布为 $\pi(\mathbf{x})$ 。Gibbs Sampling 每一步更新一个坐标 i , 从条件分布 $\pi(x'_i | \mathbf{x}_{-i})$ 采样新值 x'_i , 其中 $\mathbf{x}_{-i} = (x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_d)$ 。新状态为 $\mathbf{x}' = (x_1, \dots, x_{i-1}, x'_i, x_{i+1}, \dots, x_d)$, 满足 $\mathbf{x}_{-i} = \mathbf{x}'_{-i}$ 。转移概率 $P(\mathbf{x} \rightarrow \mathbf{x}') = \pi(x'_i | \mathbf{x}_{-i})$ 。下证其满足细致平衡条件: $\pi(\mathbf{x})P(\mathbf{x} \rightarrow \mathbf{x}') = \pi(\mathbf{x}')P(\mathbf{x}' \rightarrow \mathbf{x})$ 。注意到:

$$LHS = \pi(\mathbf{x})\pi(x'_i | \mathbf{x}_{-i}) = \frac{\pi(\mathbf{x})\pi(\mathbf{x}')}{\pi(\mathbf{x}_{-i})}$$

右边:

$$RHS = \pi(\mathbf{x}')\pi(x_i | \mathbf{x}'_{-i}) = \pi(\mathbf{x}')\pi(x_i | \mathbf{x}_{-i}) = \frac{\pi(\mathbf{x}')\pi(\mathbf{x})}{\pi(\mathbf{x}_{-i})}$$

因此 $LHS = RHS$, 吉布斯采样满足细致平衡条件。