一、观察值缺失时均值向量的推断

人们通常得不到观察向量的某些分量值，到目前为止，还没有能够处理这种情形的统计方法。`Dempster`等人在1977年提出从不完全数据出发计算极大似然估计的一般方法。这种方法通常被称为EM算法，该方法包含两个迭代计算组成，她们分别称为预测步骤和估计步骤：

预测步骤： 给定未知参数的某一估计，预测任何缺失观测值对（完全数据）充分统计量的贡献。

估计步骤： 利用预测得到的充分统计量计算参数的修正估计。

1.1 理论推导

观测值$x_1,x_2,\dots,x_n\sim N_p(\mu,\Sigma)$，另外$(n-1)S=\sum_{i=1}^n(x_i-\hat{x})(x_i-\hat{x})^\top$

$$
\begin{aligned}
T_1&=\sum_{i=1}^n x_i=n\bar{x}\\
T_2&=\sum_{i=1}^n x_ix_i^\top\\
&=\sum_{i=1}^n(x_i-\bar{x}+\bar{x})(x_i-\bar{x}+\bar{x})^\top\\
&=\sum_{i=1}^n(x_i-\bar{x})(x_i-\bar{x})^\top+\sum_{i=1}^n(x_i-\bar{x})\bar{x}^\top+\sum_{i=1}^n\bar{x}(x_i-\bar{x})^\top+\sum_{i=1}^n\bar{x}\bar{x}^\top\\
&=\sum_{i=1}^n(x_i-\bar{x})(x_i-\bar{x})^\top+0+0+n\bar{x}\bar{x}^\top\\
&=(n-1)S+n\bar{x}\bar{x}^\top
\end{aligned}
$$

对每一具有缺损值得向量x_j，记$x_j^{(1)}$为其缺损向量，$x_j^{(2)}$为其可获得分量，于是

$$
x_j=\begin{bmatrix}x_j^{(1)}\\ \dots\\ x_j^{(2)}\end{bmatrix},\mu=\begin{bmatrix}\mu^{(1)}\\ \dots\\ \mu^{(2)}\end{bmatrix},\Sigma=\begin{bmatrix}\Sigma_{11}&\Sigma_{12}\\ \\ \Sigma_{21}&\Sigma_{22}\end{bmatrix}
$$

- 证明分块矩阵求行列式

  $$
  \begin{bmatrix}I&0\\-A_{21}A_{11}^{-1}&I\end{bmatrix}\begin{bmatrix}A_{11}&A_{12}\\A_{21}&A_{22}\end{bmatrix}=\begin{bmatrix}A_{11}&A_{12}\\0&A_{22}-A_{21}A_{11}^{-1}A_{12}\end{bmatrix}
  $$

  两边取行列式：

  $$
  |A|=|A_{11}||A_{22}-A_{21}A_{11}^{-1}A_{12}|
  $$

  $$
  \begin{bmatrix}I&-\Sigma_{12}\Sigma_{22}^{-1}\\0&I\end{bmatrix}\begin{bmatrix}\Sigma_{11}&\Sigma_{12}\\\Sigma_{21}&\Sigma_{22}\end{bmatrix}=\begin{bmatrix}\Sigma_{11}-\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}&0\\\Sigma_{21}&\Sigma_{22}\end{bmatrix}
  $$

  两边取行列式

  $$
  |A|=|A_{22}||A_{11}-A_{12}A_{22}^{-1}A_{21}|
  $$

- 证明分块矩阵求逆

  $$
  \Sigma=\begin{bmatrix}\Sigma_{11}&\Sigma_{12}\\ \\ \Sigma_{21}&\Sigma_{22}\end{bmatrix}
  $$

  $$
  \begin{bmatrix}E&-\Sigma_{12}\Sigma_{22}^{-1}\\0&E\end{bmatrix}\begin{bmatrix}\Sigma_{11}&\Sigma_{12}\\ \\ \Sigma_{21}&\Sigma_{22}\end{bmatrix}=\begin{bmatrix}\Sigma_{11}-\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}&0\\ \\ \Sigma_{21}&\Sigma_{22}\end{bmatrix}
  $$

  $$
  \begin{bmatrix}\Sigma_{11}-\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}&0\\ \\ \Sigma_{21}&\Sigma_{22}\end{bmatrix}\begin{bmatrix}E&0\\ \\ -\Sigma_{22}^{-1}\Sigma_{21}&E\end{bmatrix}=\begin{bmatrix}\Sigma_{11}-\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}&0\\ \\ 0&\Sigma_{22}\end{bmatrix}
  $$

  即，

  $$
  \begin{bmatrix}E&-\Sigma_{12}\Sigma_{22}^{-1}\\0&E\end{bmatrix}\begin{bmatrix}\Sigma_{11}&\Sigma_{12}\\ \\ \Sigma_{21}&\Sigma_{22}\end{bmatrix}\begin{bmatrix}E&0\\ \\ -\Sigma_{22}^{-1}\Sigma_{21}&E\end{bmatrix}=\begin{bmatrix}\Sigma_{11}-\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}&0\\ \\ 0&\Sigma_{22}\end{bmatrix}
  $$

  两边求逆：

$$\begin{bmatrix} E & 0 \\ -\Sigma_{22}^{-1}\Sigma_{21} & E \end{bmatrix}^{-1} \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}^{-1} \begin{bmatrix} E & -\Sigma_{12}\Sigma_{22}^{-1} \\ 0 & E \end{bmatrix} = \begin{bmatrix} \left(\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}\right)^{-1} & 0 \\ 0 & \Sigma_{22}^{-1} \end{bmatrix}$$

$$\begin{aligned} \Rightarrow \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}^{-1} &= \begin{bmatrix} E & 0 \\ -\Sigma_{22}^{-1}\Sigma_{21} & E \end{bmatrix} \begin{bmatrix} \left(\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}\right)^{-1} & 0 \\ 0 & \Sigma_{22}^{-1} \end{bmatrix} \begin{bmatrix} E & -\Sigma_{12}\Sigma_{22}^{-1} \\ 0 & E \end{bmatrix} \\ &= \begin{bmatrix} \Sigma_{11\cdot 2} & -\Sigma_{11\cdot 2}^{-1}\Sigma_{12}\Sigma_{22}^{-1} \\ -\Sigma_{22}^{-1}\Sigma_{21}\Sigma_{11\cdot 2}^{-1} & \Sigma_{22}^{-1} + \Sigma_{22}^{-1}\Sigma_{21}\Sigma_{11\cdot 2}^{-1}\Sigma_{12}\Sigma_{22}^{-1} \end{bmatrix} \end{aligned}$$

其中,

$$\Sigma_{11\cdot 2} = \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}$$

下面正式开始推导:

$$\begin{aligned} f\left(x_j^{(1)}|x_j^{(2)}\right) &= \frac{f(x_j)}{f(x_j^{(2)})} \\ &= \frac{(2\pi)^{-\frac{p}{2}}|\Sigma|^{-\frac{1}{2}}e^{-\frac{1}{2}(x_j-\mu)^\top\Sigma^{-1}(x_j-\mu)}}{(2\pi)^{-\frac{p_2}{2}}|\Sigma_{22}|^{-\frac{1}{2}}e^{-\frac{1}{2}(x_j^{(2)}-\mu^{(2)})^\top\Sigma_{22}^{-1}(x_j^{(2)}-\mu^{(2)})}} \\ &= (2\pi)^{-\frac{p_1}{2}}\left(\frac{|\Sigma|}{|\Sigma_{22}|}\right)^{-\frac{1}{2}}e^{-\frac{1}{2}\left\{\left[(x_j-\mu)^\top\Sigma^{-1}(x_j-\mu)\right]-\left[(x_j^{(2)}-\mu^{(2)})^\top\Sigma_{22}^{-1}(x_j^{(2)}-\mu^{(2)})\right]\right\}} \\ &= (2\pi)^{-\frac{p_1}{2}}\left|\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}\right|^{-\frac{1}{2}}e^{-\frac{1}{2}\left[(x_j^{(1)}-\mu^{(1)})-\Sigma_{11}\Sigma_{22}^{-1}(x_j^{(2)}-\mu^{(2)})\right]^\top(\Sigma_{11}-\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1}\left[(x_j^{(1)}-\mu^{(1)})-\Sigma_{11}\Sigma_{22}^{-1}(x_j^{(2)}-\mu^{(2)})\right]} \end{aligned}$$

其中,指数部分化简如下:$e^{-\frac{1}{2}\times E}$

$$\begin{aligned} E &= \begin{bmatrix} x_j^{(1)} - \mu^{(1)} \\ x_j^{(2)} - \mu^{(2)} \end{bmatrix}^\top \begin{bmatrix} \Sigma_{11\cdot 2} & -\Sigma_{11\cdot 2}^{-1}\Sigma_{12}\Sigma_{22}^{-1} \\ -\Sigma_{22}^{-1}\Sigma_{21}\Sigma_{11\cdot 2}^{-1} & \Sigma_{22}^{-1} + \Sigma_{22}^{-1}\Sigma_{21}\Sigma_{11\cdot 2}^{-1}\Sigma_{12}\Sigma_{22}^{-1} \end{bmatrix} \begin{bmatrix} x_j^{(1)} - \mu^{(1)} \\ x_j^{(2)} - \mu^{(2)} \end{bmatrix} - \left[(x_j^{(2)} - \mu^{(2)})\Sigma_{22}^{-1}(x_j^{(2)} - \mu^{(2)})^\top\right] \\ &= \begin{bmatrix} (x_j^{(1)} - \mu^{(1)})\Sigma_{11\cdot 2}^{-1} - (x_j^{(2)} - \mu^{(2)})\Sigma_{22}^{-1}\Sigma_{21}\Sigma_{11\cdot 2} \\ -(x_j^{(1)} - \mu^{(1)})\Sigma_{11\cdot 2}^{-1}\Sigma_{12}\Sigma_{22}^{-1} + (x_j^{(2)} - \mu^{(2)})\left(\Sigma_{22}^{-1} + \Sigma_{22}^{-1}\Sigma_{21}\Sigma_{11\cdot 2}^{-1}\Sigma_{12}\Sigma_{22}^{-1}\right) \end{bmatrix}^\top \begin{bmatrix} x_j^{(1)} - \mu^{(1)} \\ x_j^{(2)} - \mu^{(2)} \end{bmatrix} - \left[(x_j^{(2)} - \mu^{(2)})\Sigma_{22}^{-1}(x_j^{(2)} - \mu^{(2)})^\top\right] \\ &= \left[(x_j^{(1)} - \mu^{(1)})\Sigma_{11\cdot 2}^{-1} - (x_j^{(2)} - \mu^{(2)})\Sigma_{22}^{-1}\Sigma_{21}\Sigma_{11\cdot 2}\right](x_j^{(1)} - \mu^{(1)})^\top \\ &+ \left[-(x_j^{(1)} - \mu^{(1)})\Sigma_{11\cdot 2}^{-1}\Sigma_{12}\Sigma_{22}^{-1} - (x_j^{(2)} - \mu^{(2)})\left(\Sigma_{22}^{-1} + \Sigma_{22}^{-1}\Sigma_{21}\Sigma_{11\cdot 2}^{-1}\Sigma_{12}\Sigma_{22}^{-1}\right)\right](x_j^{(2)} - \mu^{(2)})^\top - \left[(x_j^{(2)} - \mu^{(2)})\Sigma_{22}^{-1}(x_j^{(2)} - \mu^{(2)})^\top\right] \\ &= (x_j^{(1)} - \mu^{(1)})\Sigma_{11\cdot 2}^{-1}(x_j^{(1)} - \mu^{(1)})^\top - (x_j^{(2)} - \mu^{(2)})\Sigma_{22}^{-1}\Sigma_{21}\Sigma_{11\cdot 2}(x_j^{(1)} - \mu^{(1)})^\top - (x_j^{(1)} - \mu^{(1)})\Sigma_{11\cdot 2}^{-1}\Sigma_{12}\Sigma_{22}^{-1}(x_j^{(2)} - \mu^{(2)})^\top \\ &+ (x_j^{(2)} - \mu^{(2)})\left(\Sigma_{22}^{-1} + \Sigma_{22}^{-1}\Sigma_{21}\Sigma_{11\cdot 2}^{-1}\Sigma_{12}\Sigma_{22}^{-1}\right)(x_j^{(2)} - \mu^{(2)})^\top - \left[(x_j^{(2)} - \mu^{(2)})\Sigma_{22}^{-1}(x_j^{(2)} - \mu^{(2)})^\top\right] \end{aligned}$$

令:

$$\begin{cases} y &= \Sigma_{12}\Sigma_{22}^{-1}(x_j^{(2)} - \mu^{(2)}) \\ y^\top &= (x_j^{(2)} - \mu^{(2)})^\top\Sigma_{22}^{-1}\Sigma_{12}^\top \end{cases}$$

那么,

$$\begin{aligned} E &= (x_j^{(1)} - \mu^{(1)})\Sigma_{11\cdot 2}^{-1}(x_j^{(1)} - \mu^{(1)})^\top - y^\top\Sigma_{11\cdot 2}^{-1}y \\ &= (x_j^{(1)} - \mu^{(1)} - y)^\top\Sigma_{11\cdot 2}^{-1}(x_j^{(1)} - \mu^{(1)} - y) \end{aligned}$$

所以,

$$f\left(x_j^{(1)}|x_j^{(2)}\right) = (2\pi)^{-\frac{p}{2}}\left|\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}\right|^{-\frac{1}{2}}e^{-\frac{1}{2}\left[(x_j^{(1)}-\mu^{(1)})-\Sigma_{11}\Sigma_{22}^{-1}(x_j^{(2)}-\mu^{(2)})\right]^\top(\Sigma_{11}-\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1}\left[(x_j^{(1)}-\mu^{(1)})-\Sigma_{11}\Sigma_{22}^{-1}(x_j^{(2)}-\mu^{(2)})\right]}$$

$$\Rightarrow \begin{cases} \widetilde{x_j^{(1)}} &= \widetilde{\mu^{(1)}} + \Sigma_{12}\Sigma_{22}^{-1}(x_j^{(2)} - \mu^{(2)}) & \to T_1 \\ x_j^{(1)}\widetilde{(x_j^{(1)})}^\top &= x_j^{(1)}\widetilde{(x_j^{(1)})}^\top + (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}) & \to T_2 \\ x_j^{(2)}\widetilde{(x_j^{(2)})}^\top &= \widetilde{x_j^{(2)}}\,(x_j^{(1)})^\top & \to T_2 \end{cases}$$

修正后的极大似然估计:

$$\begin{cases} \widetilde{\mu} &= \frac{1}{n}\widetilde{T_1} \\ \widetilde{\Sigma} &= \frac{1}{n}\widetilde{T_2} - \widetilde{\mu}\widetilde{\mu}^\top \end{cases}$$

1.2 代码

EM算法代码如下。

```
def em(xdata, mu0, Sigma0, times = 0):
    time = 0
    n, p = xdata.shape
    mu1 = mu0 + 1
    Sigma1 = Sigma0 + 1

    # 计算均方误差，前后两次迭代的均值和协方差元素逐个比较
    def err(mu0, Sigma0, mu1, Sigma1):
        th0 = np.concatenate((mu0, Sigma0.flatten()))
        th1 = np.concatenate((mu1, Sigma1.flatten()))
        return np.sqrt(np.sum((th0 - th1) ** 2))

    if times:
        # 循环迭代
        while time < times:
            time += 1
            mu1 = mu0.copy()
            Sigma1 = Sigma0.copy()

            # T_1
            T_1 = np.copy(xdata)
            # T_2的增量
            delta = np.zeros((p, p))

            # 迭代每一组数据
            for i in range(n):
                # 如果这一行数据有缺失值，才继续循环
                if np.any(np.isnan(xdata[i])):
                    # 拿到这一行数据
                    zi = xdata[i]
                    # 找到缺失值的索引
                    na_idx = np.where(np.isnan(zi))[0]
                    # 找到非缺失值的索引
                    cs_idx = np.where(~np.isnan(zi))[0]

                    # 分块
                    Sigma011 = Sigma0[np.ix_(na_idx, na_idx)]
                    Sigma012 = Sigma0[np.ix_(na_idx, cs_idx)]
                    Sigma022_iv = np.linalg.inv(Sigma0[np.ix_(cs_idx, cs_idx)])

                    T_1[i, na_idx] = mu0[na_idx] + np.dot(Sigma012, Sigma022_iv).dot(zi[cs_idx] - mu0[cs_idx])
                    delta[np.ix_(na_idx, na_idx)] += Sigma011 - np.dot(Sigma012, Sigma022_iv).dot(Sigma012.T)

            mu0 = np.mean(T_1, axis=0)
            # T_2 = (n - 1) * np.cov(T_1, rowvar=False) + delta +  n * np.dot(mu0, mu0.T)
            # Sigma0 = T_2 / n - np.dot(mu0, mu0.T)
            # 上面两步合并为下面一步
            Sigma0 = (n - 1) * np.cov(T_1, rowvar=False) / n + delta / n
    else:
        # 循环迭代
        while err(mu0, Sigma0, mu1, Sigma1) > 1e-12:
            mu1 = mu0.copy()
            Sigma1 = Sigma0.copy()

            # T_1
            T_1 = np.copy(xdata)
            # T_2的增量
            delta = np.zeros((p, p))

            # 迭代每一组数据
            for i in range(n):
                # 如果这一行数据有缺失值，才继续循环
                if np.any(np.isnan(xdata[i])):
                    # 拿到这一行数据
                    zi = xdata[i]
                    # 找到缺失值的索引
                    na_idx = np.where(np.isnan(zi))[0]
```

```
                    # 找到非缺失值的索引
                    cs_idx = np.where(~np.isnan(zi))[0]

                    # 分块
                    Sigma011 = Sigma0[np.ix_(na_idx, na_idx)]
                    Sigma012 = Sigma0[np.ix_(na_idx, cs_idx)]
                    Sigma022_iv = np.linalg.inv(Sigma0[np.ix_(cs_idx, cs_idx)])

                    T_1[i, na_idx] = mu0[na_idx] + np.dot(Sigma012, Sigma022_iv).dot(zi[cs_idx] - mu0[cs_idx])
                    delta[np.ix_(na_idx, na_idx)] += Sigma011 - np.dot(Sigma012, Sigma022_iv).dot(Sigma012.T)

            mu0 = np.mean(T_1, axis=0)
            # T_2 = (n - 1) * np.cov(T_1, rowvar=False) + delta +  n * np.dot(mu0, mu0.T)
            # Sigma0 = T_2 / n - np.dot(mu0, mu0.T)
            # 上面两步合并为下面一步
            Sigma0 = (n - 1) * np.cov(T_1, rowvar=False) / n + delta / n

    return {'mu': mu0, 'Sigma': Sigma0}
```

1.3 结果

1.3.1 验证算法的正确性

为了验证代码的正确性，我用例5.13的数据，设置EM算法只迭代一次观察结果。

```
jun = np.array([6, 1, 4])
matrix = np.array([
    [np.nan, 0, 3],
    [7, 2, 6],
    [5, 1, 2],
    [np.nan, np.nan, 5]
])

S = np.array([
    [0.5, 0.25, 1],
    [0.25, 0.5, 0.75],
    [1, 0.75, 2.5]
])

result2 = em(matrix, jun, S, 10)
print(result2['mu'])
print(result2['Sigma'])
```

```
估计 mu:
[6.03181818 1.075      4.        ]
估计 Sigma:
[[0.60530992 0.33329545 1.16818182]
 [0.33329545 0.585625   0.825     ]
 [1.16818182 0.825      2.5       ]]
```

如图所示，代码运行出来的结果与例教材5.13迭代一次的结果相符。

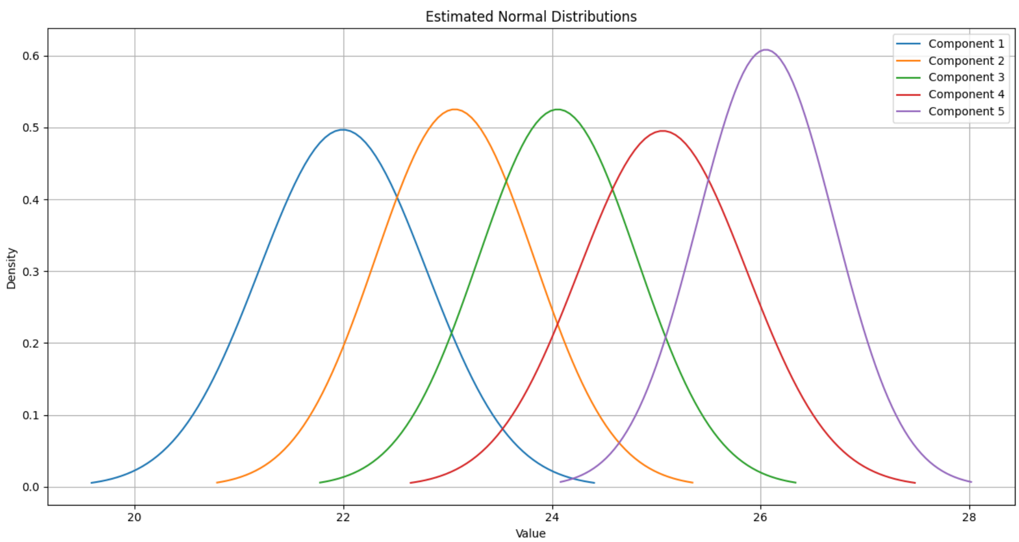
1.3.2 生成正态分布的数据运行EM算法

```
# 设置超参数
np.random.seed(1422)
mu0 = np.array([22, 23, 24, 25, 26])
p = 5
n = 1000
Sig0 = np.array([
    [ 0.64422976,  0.02235931,  0.00341657,  0.03159973, -0.11107787],
    [ 0.02235931,  0.55234995, -0.07244604,  0.12820811,  0.23877859],
    [ 0.00341657, -0.07244604,  0.64107747,  0.02788362, -0.06677286],
    [ 0.03159973,  0.12820811,  0.02788362,  0.67289534,  0.06010743],
    [-0.11107787,  0.23877859, -0.06677286,  0.06010743,  0.44281487],
])
# 生成指定均值和协方差的数据
triv = np.random.multivariate_normal(mu0, Sig0, n)
```

```python
# 随机缺失
misp = 0.2
misidx = np.random.binomial(1, misp, size=(n, p)).astype(bool)
triv[misidx] = np.nan

com_cases = triv[~np.isnan(triv).any(axis=1)]

# 初始化EM算法参数
mu_ini = np.zeros(p)
Sigma_ini = np.eye(p)

# EM 估计
result = em(com_cases, mu_ini, Sigma_ini)
print("估计 mu:")
print(result['mu'])
print("估计 Sigma:")
print(result['Sigma'])

# 画出正态分布图
plt.figure(figsize=(12, 8))
for i in range(p):
    mean = result['mu'][i]
    cov = result['Sigma'][i, i]  # 取对角元素作为方差

    x = np.linspace(mean - 3*np.sqrt(cov), mean + 3*np.sqrt(cov), 100)
    plt.plot(x, multivariate_normal.pdf(x, mean=mean, cov=cov), label=f'Component {i+1}')

plt.title('Estimated Normal Distributions')
plt.xlabel('Value')
plt.ylabel('Density')
plt.legend()
plt.grid(True)
plt.show()
```

```
估计 mu:
[21.99568816 23.06858087 24.05570571 25.0617277  26.04997606]
估计 Sigma:
[[ 0.64430053  0.01062539  0.06854223  0.02172672 -0.0666111 ]
 [ 0.01062539  0.57667491 -0.02605814  0.1324928   0.24202908]
 [ 0.06854223 -0.02605814  0.57688668  0.0653542  -0.04990927]
 [ 0.02172672  0.1324928   0.0653542   0.6486707   0.1256597 ]
 [-0.0666111   0.24202908 -0.04990927  0.1256597   0.4300725 ]]
```

画出的正态分布图如下：



二、验证巴特利特关于多元方差分析的抽样分布定理

2.1 理论推导

设从n个总体分别抽取的随机样本为

$$\begin{gathered}\text{总体1：}X_{11}, X_{12}, \cdots, X_{1n}\\ \text{总体2：}X_{21}, X_{22}, \cdots, X_{2n}\\ \vdots\\ \text{总体g：}X_{g1}, X_{g2}, \cdots, X_{gn}\end{gathered}$$

处理效应的平方和：

$$B=\sum_{l=1}^{g} n_l(\overline{x_l}-\overline{x})(\overline{x_l}-\overline{x})^T$$

残差平方和：

$$W=\sum_{l=1}^{g}\sum_{j=1}^{n_l}(x_{lj}-\overline{x_l})(x_{lj}-\overline{x_l})^T$$

则

$$\Lambda^*=\frac{|W|}{|B+W|}=\frac{|\sum_{l=1}^{g}\sum_{j=1}^{n_l}(x_{lj}-\overline{x_l})(x_{lj}-\overline{x_l})^T|}{|\sum_{l=1}^{g}\sum_{j=1}^{n_l}(x_{lj}-\overline{x})(x_{lj}-\overline{x})^T|}$$

假设$H_0:\mu_1=\mu_2=\cdots=\mu_g$，则当$H_0$为真且$\sum n_l=n$充分大，则

$$-\left(n-1-\frac{(p+g)}{2}\right)\ln\Lambda^*=-\left(n-1-\frac{(p+g)}{2}\right)\ln\left(\frac{|W|}{|B+W|}\right)$$

近似服从自由度为$p(g-1)$的χ^2分布，因此，当$\sum n_l=n$充分大时，若

$$-\left(n-1-\frac{(p+g)}{2}\right)\ln\left(\frac{|W|}{|B+W|}\right)>\chi^2_{p(g-1)}(\alpha)$$

我们就以显著性水平α拒绝H_0，其中的$\chi^2_{p(g-1)}(\alpha)$为自由度为$p(g-1)$的χ^2分布的上100α百分位数。

2.2 代码

```
from scipy.stats import norm, chi2
import numpy as np
import random
import matplotlib.pyplot as plt
import os

# 配置matplotlib以支持中文显示
plt.rcParams['font.sans-serif'] = ['SimHei']
plt.rcParams['axes.unicode_minus'] = False

# 数据生成器
def generate_dataset(count, distribution_type=None):
    if distribution_type == '正态分布':
        mean, std_dev = 0, 0.2
        return np.random.normal(loc=mean, scale=std_dev, size=count)
    elif distribution_type == '均匀分布':
        lower_bound, upper_bound = -1, 1
        return np.random.uniform(low=lower_bound, high=upper_bound, size=count)
    elif distribution_type == '泊松分布':
        lambda_param = 4
        return np.random.poisson(lam=lambda_param, size=count)
    elif distribution_type == '指数分布':
        scale_factor = 6
        return np.random.exponential(scale=scale_factor, size=count)
    elif distribution_type == 't-分布':
        degrees_of_freedom = 3
        return np.random.standard_t(df=degrees_of_freedom, size=count)
    elif distribution_type == '卡方分布':
        df_random = 5
        return np.random.chisquare(df=df_random, size=count)
    else:
```

```python
        raise ValueError('未知分布类型')

# 计算统计量
def calculate_ld_statistic(dataset, parameters_count, group_count, sample_size):
    mean_per_group = np.mean(dataset, axis=2)
    overall_mean = np.mean(mean_per_group, axis=0)

    # 计算B
    delta_matrix_1 = (mean_per_group - overall_mean[None, :])[:, :, np.newaxis]
    delta_matrix_2 = (mean_per_group - overall_mean[None, :])[:, np.newaxis, :]
    B_matrix = (delta_matrix_1 @ delta_matrix_2).sum(axis=0) * sample_size

    # 计算W
    delta_data_1 = (dataset - mean_per_group[:, :, np.newaxis]).transpose(0, 2, 1)[:, :, :, np.newaxis]
    delta_data_2 = (dataset - mean_per_group[:, :, np.newaxis]).transpose(0, 2, 1)[:, :, np.newaxis, :]
    W_matrix = (delta_data_1 @ delta_data_2).sum(axis=(0, 1))

    # 计算Lambda_star
    det_W = np.linalg.det(W_matrix)
    det_B_plus_W = np.linalg.det(B_matrix + W_matrix)
    lambda_star = det_W / det_B_plus_W

    # 计算统计量
    n = group *  sample_size
    test_statistic = -(n - 1 - (parameters_count + group_count) / 2) * np.log(lambda_star)
    return test_statistic

# 计算数据的累积分布概率
def cumulative_distribution_probabilities(data_points):
    ordered_data = np.sort(data_points)
    position_indices = np.arange(1, len(ordered_data) + 1)
    probabilities = (position_indices - 0.5) / len(ordered_data)
    return ordered_data, probabilities

# 绘制Q-Q图
def draw_qq_diagram(data_points, parameters, groups):
    degrees_of_freedom = parameters * (groups - 1)
    sorted_data, prob = cumulative_distribution_probabilities(data_points)
    normal_quantiles = chi2.ppf(prob, df=degrees_of_freedom)
    plt.scatter(sorted_data, normal_quantiles)
    plt.title(f'Q-Q图 参数p={parameters}, 组数g={groups}')
    plt.savefig(f"images/qq_plot_p_{parameters}_g_{groups}.png")
    plt.clf()

# 绘制直方图与理论分布叠加图
def overlay_histogram_and_pdf(data_points, parameters, groups):
    plt.hist(data_points, bins=60, density=True, alpha=0.6, color='blue', label='样本直方图')
    x_range = np.linspace(min(data_points), max(data_points), 10000)
    chi_squared_pdf = chi2.pdf(x_range, df=parameters * (groups - 1))
    plt.plot(x_range, chi_squared_pdf, 'red', label='卡方分布PDF')
    plt.xlabel('值')
    plt.ylabel('密度')
    plt.title(f'直方图与卡方分布 p={parameters}, g={groups}')
    plt.legend()
    plt.savefig(f"images/histogram_chi2_overlay_p_{parameters}_g_{groups}.png")
    plt.clf()

if __name__ == "__main__":
    parameter_group_combinations = [(3, 4), (4, 5), (6, 10), (8, 30)]
    sample_count = 1422
    iterations = 1422
    distribution_types = ['正态分布', '均匀分布', '泊松分布', '指数分布', 't-分布', '卡方分布']

    # 确保输出目录存在
    os.makedirs("images", exist_ok=True)

    for param, group in parameter_group_combinations:
        simulation_results = []
        for _ in range(iterations):
            all_data = []
            name_list = np.random.choice(distribution_types, size=param, replace=True)
```

```python
        for index in range(group):
            data_list = [generate_dataset(sample_count, name_list[idx])[None, :] for idx in range(param)]
            data = np.concatenate(data_list)
            all_data.append(data[None, :])

        data = np.concatenate(all_data)

        result = calculate_ld_statistic(data, param, group, sample_count)
        simulation_results.append(result)

    overlay_histogram_and_pdf(simulation_results, param, group)
    draw_qq_diagram(simulation_results, param, group)
```

2.3 结果

结果如下所示：