Mini Project 2

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Initialization: Start with initial estimates $\tilde{\boldsymbol{\mu}}$ and $\tilde{\Sigma}$.

For each observation i, partition the vector

$$oldsymbol{x}_i = egin{bmatrix} oldsymbol{x}_i^{(1)} \ oldsymbol{x}_i^{(2)} \end{bmatrix},$$

where $x_i^{(1)}$ are the *missing* components and $x_i^{(2)}$ are the *observed* components.

Similarly, partition the mean vector and covariance matrix as

$$ilde{oldsymbol{\mu}} = egin{bmatrix} ilde{oldsymbol{\mu}}^{(1)} \ ilde{oldsymbol{\mu}}^{(2)} \end{bmatrix}, \quad ilde{oldsymbol{\Sigma}} = egin{bmatrix} ilde{oldsymbol{\Sigma}}_{11} & ilde{oldsymbol{\Sigma}}_{12} \ ilde{oldsymbol{\Sigma}}_{21} & ilde{oldsymbol{\Sigma}}_{22} \end{bmatrix}.$$

E-step (Expectation): Compute the conditional expectation of the missing components:

$$ilde{oldsymbol{x}}_i^{(1)} = ilde{oldsymbol{\mu}}^{(1)} + \mathbf{B}_i \left(oldsymbol{x}_i^{(2)} - ilde{oldsymbol{\mu}}^{(2)}
ight),$$

where

$$\mathbf{B}_i = \tilde{\mathbf{\Sigma}}_{12} \tilde{\mathbf{\Sigma}}_{22}^{-1}.$$

M-step (Maximization): Update the mean and covariance estimates using the completed data $\tilde{x}_i = [\tilde{x}_i^{(1)}, x_i^{(2)}]$:

$$\tilde{\boldsymbol{\mu}}^{(new)} = \frac{1}{n} \sum_{i=1}^{n} \tilde{\boldsymbol{x}}_i, \quad \tilde{\boldsymbol{\Sigma}}^{(new)} = \frac{1}{n} \sum_{i=1}^{n} (\tilde{\boldsymbol{x}}_i - \tilde{\boldsymbol{\mu}}^{(new)}) (\tilde{\boldsymbol{x}}_i - \tilde{\boldsymbol{\mu}}^{(new)})'.$$

Repeat the E- and M-steps until convergence.

Imputation (after convergence): Once convergence is reached, with final estimates μ^* and Σ^* , generate multiple imputations as:

$$\boldsymbol{x}_{i,[m]}^{(1)} = \boldsymbol{\mu}^{*(1)} + \mathbf{B}_{i}^{*}(\boldsymbol{x}_{i}^{(2)} - \boldsymbol{\mu}^{*(2)}) + \boldsymbol{e}_{i,[m]}^{(1)},$$

where

$$\mathbf{B}_i^* = \mathbf{\Sigma}_{12}^* (\mathbf{\Sigma}_{22}^*)^{-1},$$

and

$$m{e}_{i,[m]}^{(1)} \sim \mathcal{N}_q \left(m{0}, \; m{\Sigma}_{11}^* - m{\Sigma}_{12}^* (m{\Sigma}_{22}^*)^{-1} m{\Sigma}_{21}^*
ight),$$

with q = number of missing components in observation i.

Conditional Wilk's Λ Distribution

$$\Lambda_{z|y} = rac{\Lambda_{yz}}{\Lambda_y} \sim \Lambda_{q,
u_H,
u_E-p}$$

where q=6 for length of y acids, and p=2 for length of z acids. The Wilk's Λ approximates to the following F distribution:

$$F = \frac{1 - \Lambda_{z|y}^{1/t}}{\Lambda_{z|y}^{1/t}} \frac{df_1}{df_2} \sim F_{df_1, df_2}$$

Where t = 1, $df_1 = 2$, and $df_2 = 83$.