

Expectation Maximization for fitting decision making models with Gaussian priors

- $X = \{X_i\}$: observed data, trial responses
- $Z = \{Z_i\}$: decision model parameters for all subjects
- $Z_i = \{Z_{i,d}\}$: decision model parameters for each subject, $\forall d = \{1, \dots, D\}$
- $\theta = \{\mu, \Sigma\}$: prior parameters, $\mu = \{\mu_d\}, \Sigma = \{\sigma_d^2\}, \forall d = \{1, \dots, D\}$
- $Z_i \sim N(\mu, \Sigma)$: Gaussian priors assumption
- $Z_{i,d} \sim N(\mu_d, \sigma_d^2)$: Prior parameters assumed to be independent of each other, Σ is diagonal

We are looking for the parameters of the Gaussian prior, θ , that maximize the observed data likelihood :

$$\begin{aligned}
 \theta^* &= \underset{\theta}{\operatorname{argmax}} P(X|\theta) \\
 &= \underset{\theta}{\operatorname{argmax}} \int P(X, Z|\theta) dZ \\
 &= \underset{\theta}{\operatorname{argmax}} \prod_{i=1}^N \int P(X_i, Z_i|\theta) dZ_i
 \end{aligned} \tag{1}$$

Equivalently we can solve :

$$\theta^* = \underset{\theta}{\operatorname{argmax}} \sum_{i=1}^N \ln \int P(X_i, Z_i|\theta) dZ_i \tag{2}$$

For each subject i we have :

$$\ln \int P(X_i, Z_i|\theta) dZ_i = \ln \int Q(Z_i) \frac{P(X_i, Z_i|\theta)}{Q(Z_i)} dZ_i \geq \int Q(Z_i) \ln \frac{P(X_i, Z_i|\theta)}{Q(Z_i)} dZ_i \tag{3}$$

The inequality in (3) holds by Jensen's inequality for a concave function $f(X_i, Z_i, \theta) = \frac{P(X_i, Z_i|\theta)}{Q(Z_i)}$. The equality holds only for

$$Q(Z_i) = P(Z_i|X_i, \theta) \tag{4}$$

where $P(Z_i|X_i, \theta)$ is the true posterior distribution of a subject's model parameters, given the subject's observed data X_i and the true prior parameters θ . We will approximate the posterior distribution in each iteration k of the EM algorithm, during the E-step, with $P(Z_i|X_i, \hat{\theta}_k)$.

$$\begin{aligned} \ln \int P(X_i, Z_i | \theta) dZ_i &\geq \int P(Z_i | X_i, \hat{\theta}_{k-1}) \ln \frac{P(X_i, Z_i | \theta)}{P(Z_i | X_i, \hat{\theta}_{k-1})} dZ_i \\ \Rightarrow \ln \int P(X_i, Z_i | \theta) dZ_i &\geq \int P(Z_i | X_i, \hat{\theta}_{k-1}) \ln P(X_i, Z_i | \theta) dZ_i + \int P(Z_i | X_i, \hat{\theta}_{k-1}) \ln P(Z_i | X_i, \hat{\theta}_{k-1}) dZ_i \end{aligned} \quad (5)$$

ignoring the second integral in (5), the approximate posterior entropy, as it is independent of θ , which we are optimising for, we have the expectation

$$E_{i,k} = \int P(Z_i | X_i, \hat{\theta}_{k-1}) \ln P(X_i, Z_i | \theta) dZ_i \quad (6)$$

This expectation is a lower bound on the logarithm of the marginal likelihood function (also known as model evidence) for each subject $\ln P(X_i, Z_i | \theta)$, if we first account for the offset by the approximate posterior entropy, the second integral in (5). The approximate posterior for each iteration is what is needed to complete the E-step. Here we are using the Laplace approximation, which assumes that the posterior is a Gaussian distribution. By Bayes' rule we have

$$P(Z_i | X_i, \hat{\theta}_{k-1}) = \frac{P(X_i | Z_i, \hat{\theta}_{k-1}) P(Z_i | \hat{\theta}_{k-1})}{P(X_i | \hat{\theta}_{k-1})} \quad (7)$$

and by Laplace's approximation

$$P(Z_i | X_i, \hat{\theta}_{k-1}) \sim N(m_{i,k}, \Phi_{i,k}) \quad (8)$$

$$m_{i,k} = \underset{Z_i}{\operatorname{argmax}} P(X_i | Z_i, \hat{\theta}_{k-1}) P(Z_i | \hat{\theta}_{k-1}) \quad (9)$$

$$\Phi_{i,k} = -H_{i,k}^{-1} \quad (10)$$

where $H_{i,k} = -\nabla \nabla \ln(P(X_i | Z_i, \hat{\theta}_{k-1}) P(Z_i | \hat{\theta}_{k-1}))|_{Z_i=m_{i,k}}$ is the Hessian matrix around the mode. For a derivation of (9) and (10) see [**Pattern Recognition and Machine Learning**].

After calculating the expectation (6), we are maximizing it for all subjects, during the algorithm's M-step. First, let us rewrite the expectation for one subject, then (6) becomes

$$E_{i,k} = \int P(Z_i | X_i, \hat{\theta}_{k-1}) \ln P(X_i | Z_i) dZ_i + \int P(Z_i | X_i, \hat{\theta}_{k-1}) \ln P(Z_i | \theta) dZ_i \quad (11)$$

Note that the likelihood depends only on each subject's parameters and not their priors, $P(X_i | Z_i, \theta) = P(X_i | Z_i)$. Focusing on the second integral in (11), as the only term dependent on θ we have

$$\begin{aligned} \int P(Z_i | X_i, \hat{\theta}_{k-1}) \ln P(Z_i | \theta) dZ_i &= \frac{1}{2} (D \ln 2\pi + \ln |\Sigma| + \mathcal{E}[Z_i^T \Sigma^{-1} Z_i] - \mu^T \Sigma^{-1} \mathcal{E}[Z_i] - \mathcal{E}[Z_i^T] \Sigma^{-1} \mu + \mu^T \Sigma^{-1} \mu) \\ &= \frac{1}{2} (D \ln 2\pi + \ln |\Sigma| + \operatorname{Tr}[\Sigma^{-1} (m_{i,k} m_{i,k}^T + \Phi_{i,k})] - \mu^T \Sigma^{-1} m_{i,k} - m_{i,k}^T \Sigma^{-1} \mu + \mu^T \Sigma^{-1} \mu) \end{aligned} \quad (12)$$

where $|\Sigma|$ is the determinant of the covariance matrix, Tr is the trace operation and $\mathcal{E}[Z_i] = \int Z_i P(Z_i | X_i, \hat{\theta}_{k-1}) dZ_i$ is the expectation operation under the approximate posterior. For a derivation of (12) see [**Cross entropy of Two Normal Distributions**]. To finish an iteration of EM, we are going to maximize the approximation to the original likelihood (2). Substituting (5) in (2)

$$\begin{aligned}
\theta^* \approx \hat{\theta}_k &= \operatorname{argmax}_{\theta} \sum_{i=1}^N \left[\int P(Z_i|X_i, \hat{\theta}_{k-1}) \ln P(X_i, Z_i|\theta) dZ_i + \int P(Z_i|X_i, \hat{\theta}_{k-1}) \ln P(Z_i|X_i, \hat{\theta}_{k-1}) dZ_i \right] \\
&= \operatorname{argmax}_{\theta} \sum_{i=1}^N \left[\int P(Z_i|X_i, \hat{\theta}_{k-1}) \ln P(X_i, Z_i|\theta) dZ_i \right] + \text{const}_1
\end{aligned} \tag{13}$$

now substituting (6) and then (11) into (13)

$$\hat{\theta}_k = \operatorname{argmax}_{\theta} \sum_{i=1}^N \left[\int P(Z_i|X_i, \hat{\theta}_{k-1}) \ln P(Z_i|\theta) dZ_i \right] + \text{const}_2 = \operatorname{argmax}_{\theta} \mathcal{L}(X, Z|\theta) + \text{const}_2 \tag{14}$$

where the two integrals that do not depend on θ are represented in the *const* terms. An analytical solution can be calculated for the optimal solution of (14) as

$$\frac{\partial \mathcal{L}(X, Z|\theta)}{\partial \mu} = 0 \Rightarrow \hat{\mu}_k = \frac{1}{N} \sum_{i=1}^N m_{i,k} \tag{15}$$

$$\frac{\partial \mathcal{L}(X, Z|\theta)}{\partial \Sigma} = 0 \Rightarrow \hat{\Sigma}_k = \text{diag} \left\{ \frac{1}{N} \sum_{i=1}^N (m_{i,k} m_{i,k}^T + \Phi_{i,k}) - \mu_k \mu_k^T \right\} \tag{16}$$

where $\text{diag}\{X\}$ are the diagonal elements of matrix X and $\hat{\theta}_k = \{\hat{\mu}_k, \hat{\Sigma}_k\}$.

The above process (6)-(16) is performed iteratively until $\hat{\theta}_k$ converges. For a proof of convergence of Expectation Maximization see [What is the expectation maximization algorithm? Supplementary material].

References

- Christopher M. Bishop. 2006. *Pattern Recognition and Machine Learning (Information Science and Statistics)*. Springer-Verlag, Berlin, Heidelberg.
- Cross Entropy of Two Normal Distribution, <https://www.cse.iitb.ac.in/~aruniyer/kldivergencenormal.pdf>
- Do, C., Batzoglou, S. What is the expectation maximization?. *Nat Biotechnol* 26, 897–899 (2008)