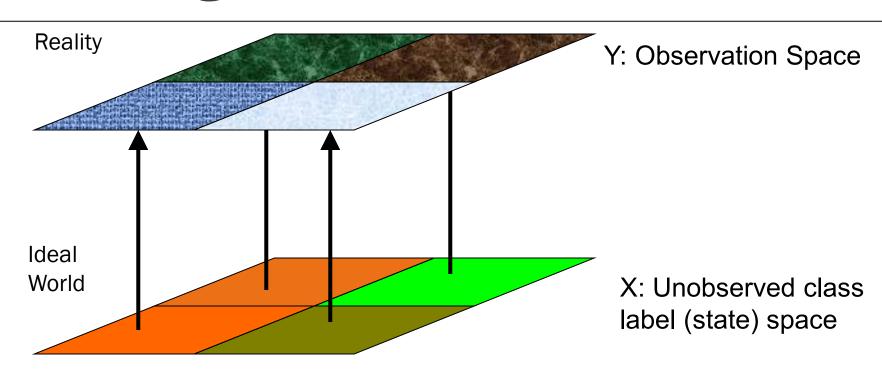


Goals

To review the missing data problem and its two major issues

To introduce a soft-clustering algorithm, i.e., Expectation Maximization (EM) algorithm.

Missing Data Problem Restatement



Mapping $X \to Y$ loses the class label information.

Inference $Y \to X$ is needed.

Some Review of Probability Theory

Where do we start?

$$\alpha_i = p_X(x = i)$$
 (prior probability)

$$p_{Y|X}(y|x=i) = N(y|\mu_i, \Sigma_i)$$
 (likelihood function)

Joint probability

$$p_{XY}(x,y) = p_{Y|X}(y|x)p_X(x)$$

Bayes' Law of posteriori probability

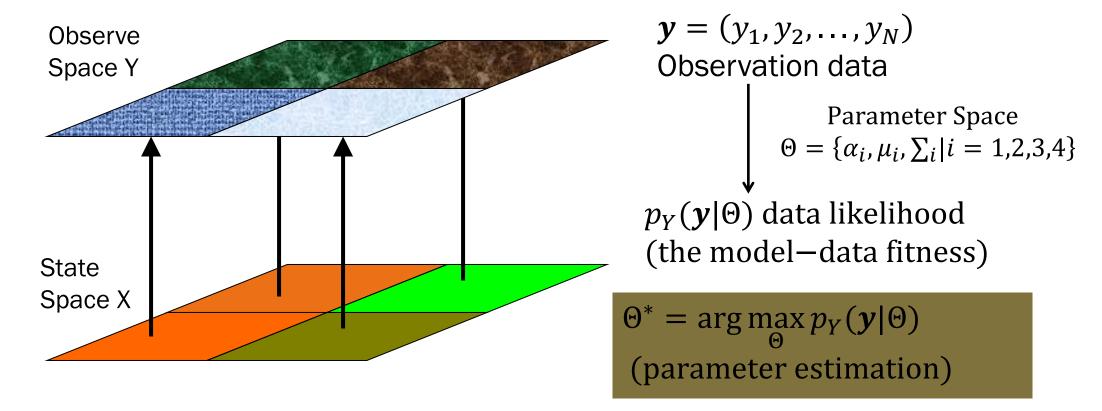
$$p_{X|Y}(x|y) = \frac{p_{XY}(x,y)}{p_Y(y)} = \frac{p_{Y|X}(y|x)p_X(x)}{p_Y(y)}$$

Y: observation (e.g., symptoms)

X: label (e.g., diseases)

Marginalization probability $p_Y(y) = \sum_{x} p_{XY}(x, y) = \sum_{x} p_{Y|X}(y|x) p_X(x)$

Issue (1) Parameter Estimation



To find the parameter Θ that can best explain the current observation y.

Formulation: Parameter Estimation

How does a tailor make a cloth?

To make a cloth that fits best to the body

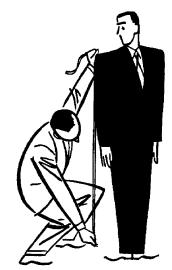
How to estimate the parameters Θ ?

• Estimating Θ that best fits the data set $\mathbf{y} = (y_1, y_2, \dots, y_N)$.

How to evaluate the fitness between Θ and y?

 \circ The fitness between Θ (model) and y (data) is reflected by the likelihood of y given Θ . Therefore, parameter estimation is:

$$\Theta^* = \arg \max_{\Theta} p_Y(\mathbf{y}|\Theta) = \arg \max_{\Theta} \prod_{i=1}^{N} p_Y(y_i|\Theta) = \arg \max_{\Theta} \sum_{i=1}^{N} \log(p_Y(y_i|\Theta))$$



Issue (2) Data Classification

To classify data, we need to compute the probability of data sample y belonging to class x, i.e., the posterior probability p(x|y), which is computed during parameter estimation.

$$\alpha_i = p_X(x=i) \qquad p_{Y|X}(y|x=i) = N(y|\mu_i, \Sigma_i)$$
 (prior probability) (likelihood function)
$$p_{X|Y}(x|y) = \frac{p_{XY}(x,y)}{p_Y(y)} = \frac{p_{Y|X}(y|x)p_X(x)}{\sum_{i=1}^k p_{Y|X}(y|x=i)p_X(x=i)}$$
 (posterior probability)

(Bayes' law)

 $x^* = \arg_{x \in X} \max p_{X|Y}(x|y)$ (maximum *a posteriori* or MAP)

Data Classification Example

If we have six samples and three classes, the missing data indicates the class label for each pixel. Hopefully, the estimated missing data will be close it.

$$\mathbf{I}^{0} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}_{6 \times 3}$$

The true missing data

$$\mathbf{I} = \begin{bmatrix} 0.1 & 0.8 & 0.1 \\ 0.3 & 0.6 & 0.1 \\ 0.4 & 0.3 & 0.3 \\ 0.7 & 0.2 & 0.1 \\ 0.3 & 0.2 & 0.5 \\ 0.05 & 0.05 & 0.9 \end{bmatrix}_{6\times}^{6\times}$$

$$x_l = \arg_{m \in \{1, \dots, g\}} \max \mathbf{I}(l, m)$$

The estimated missing data

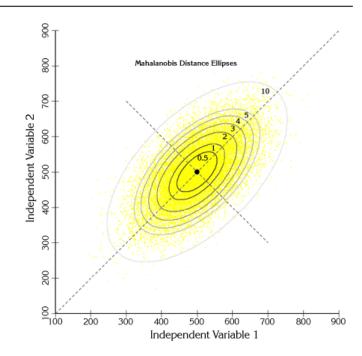
EM Formulation: Likelihood Function

What is a likelihood function?

- The likelihood function indicates how likely a particular distribution is to produce an observed sample. It is like a ruler for the tailor.
- For cluster i, we can assume a d-dimensional Gaussian PDF as the likelihood function of data samples in that class that is defined by mean μ_i and covariance matrix Σ_i

$$p_{Y|X}\left(y|x=i\right) = N(y|\mu_i, \Sigma_i) \qquad \qquad \underline{\text{Mahalanobis Distance}}$$

$$p_Y(y|\theta_i) = \frac{1}{(2\pi)^{d/2} \det(\Sigma_i)^{1/2}} \exp\left\{-\frac{1}{2}(y-\mu_i)^T \Sigma_i^{-1}(y-\mu_i)\right\}$$



Mahalanobis Distance

$$\exp\left\{-\frac{1}{2}(y-\mu_i)^T\Sigma_i^{-1}(y-\mu_i)\right\}$$

EM Formulation: Two-Step Iteration

We use a two-step iteration to solve the missing data problem

Initialize the parameters (it is like to initialize the centers in k-means)

$$\Theta = \{\alpha_i, \mu_i, \sum_i | i = 1, \dots, k\}$$

 Step 1: Estimate the missing data (x) in terms of the posterior probability of each data sample (y) (it is like to classify each data point in k-means.)

$$p_{X|Y}(x = i|y) \{i = 1,...,k\}$$

(estimate the probability of each sample belonging to different classes)

Step 2: From the estimated missing data, to obtain the maximum likelihood (ML) estimate of the parameters (it is like to update the centers in k-means)

$$\Theta^* = \arg\max_{\Theta} \log p_Y(\mathbf{y}|\Theta)$$

(update the parameters to better fit the data and the model.)

EM Algorithm: E-step

Initialization: set s=0 and

$$\Theta^0 = (\alpha_1^{(0)}, \alpha_2^{(0)}, \dots, \alpha_g^{(0)}, \theta_1^{(0)}, \theta_2^{(0)}, \dots, \theta_g^{(0)}).$$

Expectation (E-step):

Expectation (E-step):
$$I(l,m) = \frac{\alpha_m^{(s)} p_Y \left(y_l \middle| \theta_m^{(s)} \right)}{\sum_{l=1}^k \alpha_l^{(s)} p_{Y|X} \left(y_l \middle| \theta_l^{(s)} \right)} = p_{X|Y} (x_l = m | y_l, \underline{\Theta}^{(s)})$$

$$= \frac{p_{X|Y}(x = i | y)}{\sum_{l=1}^k p_{Y|X}(y | x) p_X(x)} \qquad p_{Y|X}(y_l | \theta_m^{(s)}) = \frac{\exp\left\{ -\frac{1}{2} (y_l - \mu_m)^T \sum_{m}^{-1} (y_l - \mu_m) \right\}}{(2\pi)^{d/2} \det(\Sigma_l)^{1/2}}$$

EM Algorithm: M-step

Maximization (M-step): $\Theta^* = \arg \max_{\Theta} \log p(y|\Theta)$ $\alpha_m^{(s+1)} = p_X(x) = \frac{1}{N} \sum_{l=1}^{N} p_{X|Y}(x_l = m|y_l, \Theta^{(s)})$ $\theta_{m}^{(s+1)} = \frac{\sum_{l=1}^{N} y_{l} \cdot p_{X|Y}(x_{l} = m|y_{l}, \Theta^{(s)})}{\sum_{l=1}^{N} p_{X|Y}(x_{l} = m|y_{l}, \Theta^{(s)})}$ $\Sigma_{m}^{(s+1)} = \frac{\sum_{l=1}^{N} p_{X|Y}(x_{l} = m|y_{l}, \Theta^{(s)}) \left\{ (y_{l} - \mu_{m}^{(s)})(y_{l} - \mu_{m}^{(s)})^{T} \right\}}{\sum_{l=1}^{N} p_{X|Y}(x_{l} = m|y_{l}, \Theta^{(s)})}$