Essential Estimation Techniques in Data Science

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Point Estimation

In **point estimation**, we estimate an unknown parameter of the population using a single number that is calculated from the sample data which is a subset of the population.

Example

Based on sample results, we estimate that p, the proportion of all Indian Voters who are in favor of a particular party, is 0.6.

Maximum Likelihood Estimation (MLE)

In the maximum likelihood estimation (MLE) the parameters of a probability distribution are estimated by maximizing a likelihood function, so that under the assumed statistical model the observed data is most probable.

Mathematically, let $X_1, X_2, \cdots, X_n$ be a random sample from a population with density function f and unknown parameter θ. The MLE of θ is such that

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}}\, f(\theta | x_1, x_2, \ldots, x_n).$$

MLE for Bernoulli distribution

- Data = $\{H, T, T, T, H, \ldots\}$.
- $\mathbb{P}(\textit{Heads}) = p$ and $\mathbb{P}(\textit{Tails}) = 1 - p$, where p is unknown parameter.
- MLE: Choose p that maximizes the probability of observed data, that is

$$\begin{aligned}
\hat{p} &= \operatorname*{argmax}_p \mathbb{P}(\textit{Data}|p) \\
&= \operatorname*{argmax}_p \mathbb{P}(x_1, x_2, \ldots, x_n|p) \\
&= \operatorname*{argmax}_p p^{\sum_{i=1}^n x_i}(1-p)^{n-\sum_{i=1}^n x_i} \\
&= \frac{\sum_{i=1}^n x_i}{n} = \bar{x}.
\end{aligned}$$

Thus, the MLE for p is the ratio of number of heads with the total number of trials.

Simple Linear Regression parameters estimation using MLE

Our data are (x_i, y_i) having n observations with one explanatory variable and one response variable. The model is

$$y_i = \alpha + \beta x_i + \epsilon_i, \quad \epsilon_i \sim \mathit{Normal}(0, \sigma^2).$$

The likelihood function is

$$\begin{aligned} L(\alpha, \beta, \sigma^2 | x, y) &= \frac{1}{\sigma^n (2\pi)^{n/2}} e^{-\frac{1}{2\sigma^2} \sum_{i=1}^n \epsilon_i^2} \\ &= \frac{1}{\sigma^n (2\pi)^{n/2}} e^{-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \alpha - \beta x_i)^2}. \end{aligned}$$

The log-likelihood function is

$$\begin{aligned} l(\alpha, \beta, \sigma^2 | x, y) &= \log L(\alpha, \beta, \sigma^2 | x, y) \\ &= -n \log(\sigma) - \frac{n}{2} \log(2\pi) - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \alpha - \beta x_i)^2. \end{aligned}$$

Regression parameters estimation using MLE contd...

Thus, maximizing the likelihood function for the parameters α and β is equivalent to minimizing

$$S(\alpha, \beta) = \sum_{i=1}^{n} (y_i - \alpha - \beta x_i)^2.$$

The parameters can be obtained by differentiating S with respect to α and β and putting these equations equal to 0.

AR(1) parameters estimation using MLE

- A stationary Gaussian process has the form

$$X_t = c + \rho X_{t-1} + \epsilon_t, \ t = 1, 2, \cdots, \text{ where } |\rho| < 1.$$

- $\mathbb{E}X_1 = \frac{1}{1-\rho}$ and $\text{Var}(X_1) = \frac{\sigma^2}{1-\rho^2}$.
- The errors are Gaussian and hence $X_1 \sim N\left(\frac{c}{1-\rho}, \frac{\sigma^2}{1-\rho^2}\right)$.
- $X_2 = c + \rho X_1 + \epsilon_2$, and hence $(X_2|X_1 = x_1) \sim N\left(c + \rho x_1, \sigma^2\right)$
- Similarly, $X_3 = c + \rho X_2 + \epsilon_3$, and hence $(X_3|X_2 = x_2, X_1 = x_1) = (X_3|X_2 = x_2) \sim N\left(c + \rho x_2, \sigma^2\right)$.
- The likelihood of the complete sample can thus be calculated as

$$f_{X_n, X_{n-1}, X_{n-2}, \cdots, X_1}(x_n, x_{n-1}, x_{n-2}, \cdots, x_1) = f_{X_1}(x_1) \prod_{j=2}^{n} f_{X_j|X_{j-1}}(x_j|x_{j-1}$$

Least Square Estimation

Least Square Estimation

Suppose, we have a data set $(x_i, y_i), i = 1, 2, \cdots, n$ and we are interested to fit a best function f such that

$$y_i = f(x_i) + \epsilon_i,$$

which describes the relationship between y_i and x_i. We can use the following steps:

- Define the model depending on your data. For example $y_i = f(x_i) + \epsilon_i$.
- Formulate the least square problem by minimizing the residual square i.e.

$$S = \sum_{i=1}^{n} (y_i - f(x_i))^2.$$

Least square estimation contd...

Many times we use parametric model for example $y_i = \alpha + \beta X_i + \epsilon_i$. Then, the least square estimation become to estimate α and β which minimizes

$$S = \sum_{i=1}^{n} (y_i - \alpha - \beta x_i)^2.$$

We also consider the multiple linear regression in the matrix form

$$Y = AX + \epsilon.$$

Weighted Least Square

WLS

- The linear regression model is

$$y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \epsilon_i,$$

  where the random errors are iid $N(0, \sigma^2)$.

- What happens if the ϵ_i's are independent but with unequal variance i.e. $\epsilon_i \sim N(0, \sigma_i^2)$? Also called heteroscedasticity.

- The ordinary least squares (OLS) estimates for β_j are unbiased, but no longer have the minimum variance.

- The weighted Least Squares (WLS) fixes the problem of heteroscedasticity

WLS

- For the model

$$y_i = \beta_0 + \beta_1 1 x_{i1} + \cdots + \beta_p x_{ip} + \epsilon_i,$$

where $\epsilon_i \sim N(0, \sigma_i^2)$?.

- The weighted Least Squares (WLS) is finding the estimates of β_j such that

$$L(\beta_0, \beta_1, \cdots, \beta_p) = \sum_{i=1}^{n} \frac{(y_i - \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip})^2}{\sigma_i^2}.$$

- In WLS, we focus more on minimizing errors of observation with smaller variances and focus less on minimizing errors of observations with larger variances.

- In general WLS is finding the estimates of β_j such that

$$L(\beta_0, \beta_1, \cdots, \beta_p) = \sum_{i=1}^{n} w_i (y_i - \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip})^2,$$

where the weights $w_1, w_2, \cdots, w_n$ are known and $w_i > 0$ for

WLS estimates

The WLS estimates of β_j which minimize

$$L(\beta_0, \beta_1, \cdots, \beta_p) = \sum_{i=1}^{n} w_i (y_i - \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip})^2,$$

is

$$\hat{\beta}_{WLS} = (X^T W X)^{-1} X^T W Y,$$

where

$$Y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}, X = \begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{pmatrix}, W = \begin{pmatrix} w_1 & 0 & 0 & \cdots & 0 \\ 0 & w_2 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & w_n \end{pmatrix}$$

Maximum A Posteriori Estimation

Bayesian Statistics

being, relating to, or involving statistical methods that assign probabilities or distributions to events (such as rain tomorrow) or parameters (such as a population mean) based on experience or best guesses before experimentation and data collection and that apply Bayes' theorem to revise the probabilities and distributions after obtaining experimental data

- Webster's Revised Unabridged Dictionary

Prior/Posterior

Example

Suppose you have 4 coins. Three of them are fair coins but the fourth is a weighted coin which has 80% chance of landing heads up. You take a coin randomly out of your pocket and toss it. Suppose it lands heads up. What is the probability that the coin is the weighted coin ?

Prior: π(fair) = 0.75, π(weighted) = 0.25.
Likelihood: $\mathbb{P}$(head|fair) = 0.5 and $\mathbb{P}$(head|weighted) = 0.8.
Posterior:

$$\mathbb{P}(\textit{weighted}|\textit{head}) = \frac{\mathbb{P}(\textit{head}|\textit{weighted})\mathbb{P}(\textit{weighted})}{\mathbb{P}(\textit{head}|\textit{fair})\mathbb{P}(\textit{fair}) + \mathbb{P}(\textit{head}|\textit{weighted})\mathbb{P}(\textit{weigh}}$$
$$= 0.348.$$

Bayesian Inference

Prior

The prior is the probability distribution that represents your uncertainty over θ **before** you have sampled any data.

Posterior

The posterior is the probability distribution that represents your uncertainty over θ **after** you have sampled data.

We have

$$\pi(\Theta|X) = \frac{f_{X|\Theta}(x|\theta)\pi_\Theta(\theta)}{f_X(x)}.$$

Classical vs Bayesian Statistics

Classical Statistics

In classical statistics, the unknown parameter is a fixed constant, just we don't know it.

Bayesian Statistics

In Bayesian statistics, the unknown parameter is assumed to be a random variable.

Different representations

Discrete parameter discrete data

$$p_{\Theta|X}(\theta|x) = \frac{p_{X|\Theta}(x|\theta)p_{\Theta}(\theta)}{p_X(x)}$$

Discrete parameter continuous data

$$p_{\Theta|X}(\theta|x) = \frac{f_{X|\Theta}(x|\theta)p_{\Theta}(\theta)}{f_X(x)}$$

Continuous parameter discrete data

$$f_{\Theta|X}(\theta|x) = \frac{p_{X|\Theta}(x|\theta)f_{\Theta}(\theta)}{p_X(x)}$$

Example

Example

Find the posterior distribution of probability of heads denoted by θ on a coin. Suppose x heads are observed in n tosses.
Solution: Suppose we assume a uniform prior for Θ i.e. $f_\Theta(\theta) = 1,\ 0 < \theta < 1$. Also

$$p_{X|\Theta}(x|\theta) = \binom{n}{x}\theta^x(1-\theta)^{n-x}.$$

We then have

$$\begin{aligned} f_{\Theta|X}(\theta|x) &= \frac{\binom{n}{x}\theta^x(1-\theta)^{n-x}}{\int_0^1 \binom{n}{x}\theta^x(1-\theta)^{n-x}d\theta} \\ &= \frac{(n+1)!\theta^x(1-\theta)^{n-x}}{x!(n-x)!}. \end{aligned}$$

Maximum a posteriori probability (MAP) Estimator

We choose the estimator $\hat{\Theta}$ such that posterior probability $p_{\Theta|X}(\theta|x)$ or $f_{\Theta|X}(\theta|x)$ is maximize. In other words the MAP estimate of θ is

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}}\, f_{\Theta|X}(\theta|x) \text{ or } \underset{\theta}{\operatorname{argmax}}\, p_{\Theta|X}(\theta|x).$$

Example

In the coin toss example, the MAP estimate will be

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}}\, \frac{(n+1)!\theta^x(1-\theta)^{n-x}}{x!(n-x)!} = \frac{x}{n},$$

which is same as the maximum likelihood estimate (MLE).

Example

Let X be a continuous random variable with the following pdf

$$f_X(x) = \begin{cases} 2x \text{ if } 0 < x < 1 \\ 0 \quad \text{otherwise} \end{cases}$$

Also, suppose that

$$Y|X = x \sim \text{Geometric}(x).$$

Find the MAP estimate of X given $Y = 3$.
Hint: $p_{Y|X}(y|x) = x(1-x)^{y-1},\ y = 1, 2, \cdots$

MAP estimation: Gaussian distribution

Example

Suppose $f_\Theta(\theta) = \frac{1}{\sigma_0\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{\theta - x_0}{\sigma_0}\right)^2}$. Further, $X_1, X_2, \ldots, X_n$ which conditioned on the value $\Theta = \theta$, are independent Gaussian with mean θ and variances $\sigma_1^2, \sigma_2^2, \cdots, \sigma_n^2$. Find the MAP estimate of Θ.

Solution: We have

$$f_{X_1, X_2, \cdots, X_n}(x_1, x_2, \ldots x_n|\theta) = ce^{-\frac{1}{2}\left(\frac{x_1 - \theta}{\sigma_1}\right)^2} e^{-\frac{1}{2}\left(\frac{x_2 - \theta}{\sigma_2}\right)^2} \cdots e^{-\frac{1}{2}\left(\frac{x_n - \theta}{\sigma_n}\right)^2}.$$

Using, Bayes' theorem, we have

$$f_{\Theta|X}(\theta|x) = \frac{f_{X|\Theta}(x|\theta) f_\Theta(\theta)}{f_X(x)},$$

or

$$f_{\Theta|X}(\theta|x) \propto f_{X|\Theta}(x|\theta) f_\Theta(\theta),$$

since $f_X(x)$ is independent of θ, it doesn't play any role in

MAP estimation: Gaussian distribution contd...

$$f_{X|\Theta}(x|\theta)f_{\Theta}(\theta) = c_1 e^{-\frac{1}{2}\left(\frac{x_0-\theta}{\sigma_0}\right)^2} e^{-\frac{1}{2}\left(\frac{x_1-\theta}{\sigma_1}\right)^2} e^{-\frac{1}{2}\left(\frac{x_2-\theta}{\sigma_2}\right)^2} \cdots e^{-\frac{1}{2}\left(\frac{x_n-\theta}{\sigma_n}\right)^2}.$$

Observe that

$$e^{-\frac{1}{2}\left(\frac{x_0-\theta}{\sigma_0}\right)^2} e^{-\frac{1}{2}\left(\frac{x_1-\theta}{\sigma_1}\right)^2} = e^{-\frac{1}{2}\left(\frac{x_0^2}{\sigma_0^2}+\frac{x_1^2}{\sigma_1^2}\right)} e^{-\frac{1}{2}\left(\frac{\theta_0^2}{\sigma_0^2}+\frac{\theta_1^2}{\sigma_1^2}-2\theta\left(\frac{x_0}{\sigma_0^2}+\frac{x_1}{\sigma_1^2}\right)\right)}$$

$$= Be^{-\frac{1}{2}\frac{\left(\theta-\frac{x_0/\sigma_0^2+x_1/\sigma_1^2}{1/\sigma_0^2+1/\sigma_1^2}\right)^2}{\frac{1}{1/\sigma_0^2+1/\sigma_1^2}}},$$

which is minimize at

$$\theta = \frac{x_0/\sigma_0^2 + x_1/\sigma_1^2}{1/\sigma_0^2 + 1/\sigma_1^2}.$$

Thus MAP estimate is

$$\hat{\theta} = \frac{x_0/\sigma_0^2 + x_1/\sigma_1^2 + \cdots + x_n/\sigma_n^2}{1/\sigma_0^2 + 1/\sigma_1^2 + \cdots + 1/\sigma_n^2}.$$

EM Algorithm

Expectation Maximization Algorithm

- **Expectation-Maximization (EM)** algorithm is a general iterative algorithm for model parameter estimation by maximizing the likelihood in presence of missing data.
- An alternative to numerical optimization of the likelihood function, the EM algorithm was introduced in 1977 by Dempster, Laird and Rubin.
- Applications: Estimating Gaussian mixture models (GMMs), estimating Hidden Markov models (HMMs) and model based data clustering.

1

[1] Dempster, A.P., Laird, N.M. and Rubin, D.B. (1977). Maximum likelihood from incomplete data via EM Algorithm. J. R. Stat. Soc. Ser. B 39, 1–38.

Example: Coin Flipping

- Two coins A and B, chosen at random and flipped 10 times.
- $\mathbb{P}(\text{H from coin A}) = \theta_A$, $\mathbb{P}(\text{H from coin B}) = \theta_B$.
- Repeat the process 5 times.
- Aim: To estimate the unknown parameters θ_A and θ_B.

Example Contd...

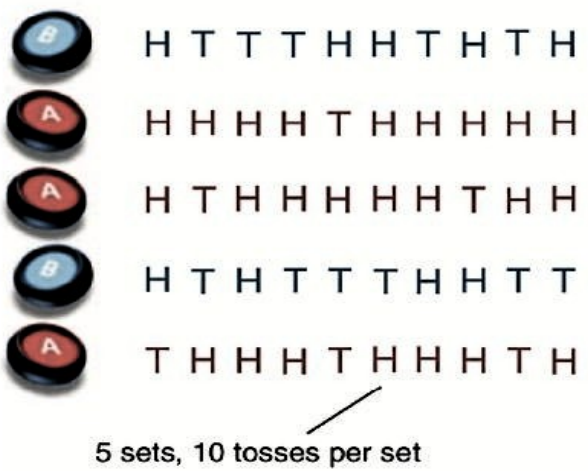
EM algorithm

$$\hat{\theta}_A = \frac{\text{\# of heads using coin A}}{\text{total \# of flips using coin A}}$$

$$\hat{\theta}_B = \frac{\text{\# of heads using coin B}}{\text{total \# of flips using coin B}}$$

Example: the 2 coin problem.
Scenario 1: no missing value:

a Maximum likelihood



Coin A	Coin B
	5 H, 5 T
9 H, 1 T	
8 H, 2 T	
	4 H, 6 T
7 H, 3 T	
24 H, 6 T	9 H, 11 T

$$\hat{\theta}_A = \frac{24}{24+6} = 0.80$$

$$\hat{\theta}_B = \frac{9}{9+11} = 0.45$$

2

[2] Do, B.C. and Batzoglou, S. (2008). What is the expectation maximization algorithm? Nature Biotechnology, 26, 897–899.

Example Contd...

Mathematically, this can be formulated as follows:

$$X_{ij} = \begin{cases} 1 & \text{if } \textit{jth} \text{ flip in the } \textit{ith} \text{ set is H} \\ 0 & \text{if } \textit{jth} \text{ flip in the } \textit{ith} \text{ set is T,} \end{cases}$$

where $1 \leq i \leq 5$ and $1 \leq j \leq 10$.

- Y_i takes value A or B based on the coin used for *ith* set.
- Let $X_i = \sum_{j=1}^{10} X_{ij}$ be the number of heads in the *ith* set.
- Also, $X_i | Y_i = k \sim \textit{Binomial}(10, \theta_k)$, where $k = \{\text{A}, \text{B}\}$.
- Based on the information, the MLEs for parameters $\hat{\theta}_A = 0.8$ and $\hat{\theta}_B = 0.45$.

MLE in presence of hidden data

- Suppose for the same dataset the coin identities are not given i.e. $Y_i's$ are hidden.
- We have “incomplete data" consisting of X values only.
- In this case, the unknown parameters can not be estimated by maximizing the likelihood or log-likelihood function.
- However, the EM algorithm first incorporates the hidden information and then maximize the expectation of the complete data log-likelihood.

Coin Flipping Example: EM algorithm

- The hidden variable $Y_i \in \{A, B\}$
- Take $\pi_A = \mathbb{P}(Y_i = A)$ and $\pi_B = \mathbb{P}(Y_i = B)$.
- Initial guess for $\pi_A^{(0)} = 0.5$, $\pi_B^{(0)} = 0.5$, $\theta_A^{(0)} = 0.6$ and $\theta_B^{(0)} = 0.5$.

- E-step: For each data X_i, compute the probabilities that it is from coin A and coin B and denote it by w_{iA} and w_{iB} respectively. That is, we guess the value of $Y_i's$ using posterior probability distribution $\mathbb{P}(Y_i = c|X_i)$, where $c \in \{A, B\}$.
- Set $w_{ic} = \mathbb{P}(Y_i = c|X_i, \theta_A^{(0)}, \theta_B^{(0)}, \pi_A^{(0)}, \pi_B^{(0)})$,

$$
\begin{aligned}
w_{ic} &= \frac{\mathbb{P}(X_i|Y_i = c)\mathbb{P}(Y_i = c)}{\mathbb{P}(X_i|Y_i = A)\mathbb{P}(Y_i = A) + \mathbb{P}(X_i|Y_i = B)\mathbb{P}(Y_i = B)} \\
&= \frac{\mathbb{P}(X_i|Y_i = c)\pi_A^{(0)}}{\mathbb{P}(X_i|Y_i = A)\pi_A^{(0)} + \mathbb{P}(X_i|Y_i = B)\pi_B^{(0)}} \qquad (1)
\end{aligned}
$$

Continued...

For set 1 i.e. $i = 1$ and coin A,

$$w_{1A} = \frac{\theta_A^{(0)5}(1-\theta_A^{(0)})^5\pi_A^{(0)}}{\theta_A^{(0)5}(1-\theta_A^{(0)})^5\pi_A^{(0)} + \theta_B^{(0)5}(1-\theta_B^{(0)})^5\pi_B^{(0)}}$$
$$= \frac{0.5 \times (0.6)^5 \times (0.4)^5}{0.5 \times (0.6)^5 \times (0.4)^5 + 0.5 \times (0.5)^5 \times (0.5)^5} \approx 0.45$$

For set 1 i.e. $i = 1$ and coin B,

$$w_{1B} = \frac{\theta_B^{(0)5}(1-\theta_B^{(0)})^5\pi_B^{(0)}}{\theta_A^{(0)5}(1-\theta_A^{(0)})^5\pi_A^{(0)} + \theta_B^{(0)5}(1-\theta_B^{(0)})^5\pi_B^{(0)}}$$
$$= \frac{0.5 \times (0.5)^5 \times (0.5)^5}{0.5 \times (0.6)^5 \times (0.4)^5 + 0.5 \times (0.5)^5 \times (0.5)^5} \approx 0.55$$

Continued...

For set 2 i.e. $i = 2$ and coin A,

$$w_{2A} = \frac{\theta_A^{(0)9}(1-\theta_A^{(0)})\pi_A^{(0)}}{\theta_A^{(0)9}(1-\theta_A^{(0)})\pi_A^{(0)} + \theta_B^{(0)9}(1-\theta_B^{(0)})\pi_B^{(0)}}$$
$$= \frac{0.5 \times (0.6)^9 \times (0.4)}{0.5 \times (0.6)^9 \times (0.4) + 0.5 \times (0.5)^9 \times (0.5)} \approx 0.80.$$

For set 2 i.e. $i = 2$ and coin B,

$$w_{2B} = \frac{\theta_B^{(0)9}(1-\theta_B^{(0)})\pi_B^{(0)}}{\theta_A^{(0)9}(1-\theta_A^{(0)})\pi_A^{(0)} + \theta_B^{(0)9}(1-\theta_B^{(0)})\pi_B^{(0)}}$$
$$= \frac{0.5 \times (0.5)^9 \times (0.5)}{0.5 \times (0.6)^9 \times (0.4) + 0.5 \times (0.5)^9 \times (0.5)}$$
$$\approx 0.2$$

Continued...

- M-step: Now, we use the membership weights from E-step to update new parameter values.
- Let $n_A = w_{1A} + w_{2A}$ and $n_B = w_{1B} + w_{2B}$.
- Update the parameters as follows:

$$\pi_A^{(1)} = \frac{n_A}{n} = \frac{1.25}{2}$$
$$\pi_B^{(1)} = \frac{n_B}{n} = \frac{0.75}{2}.$$

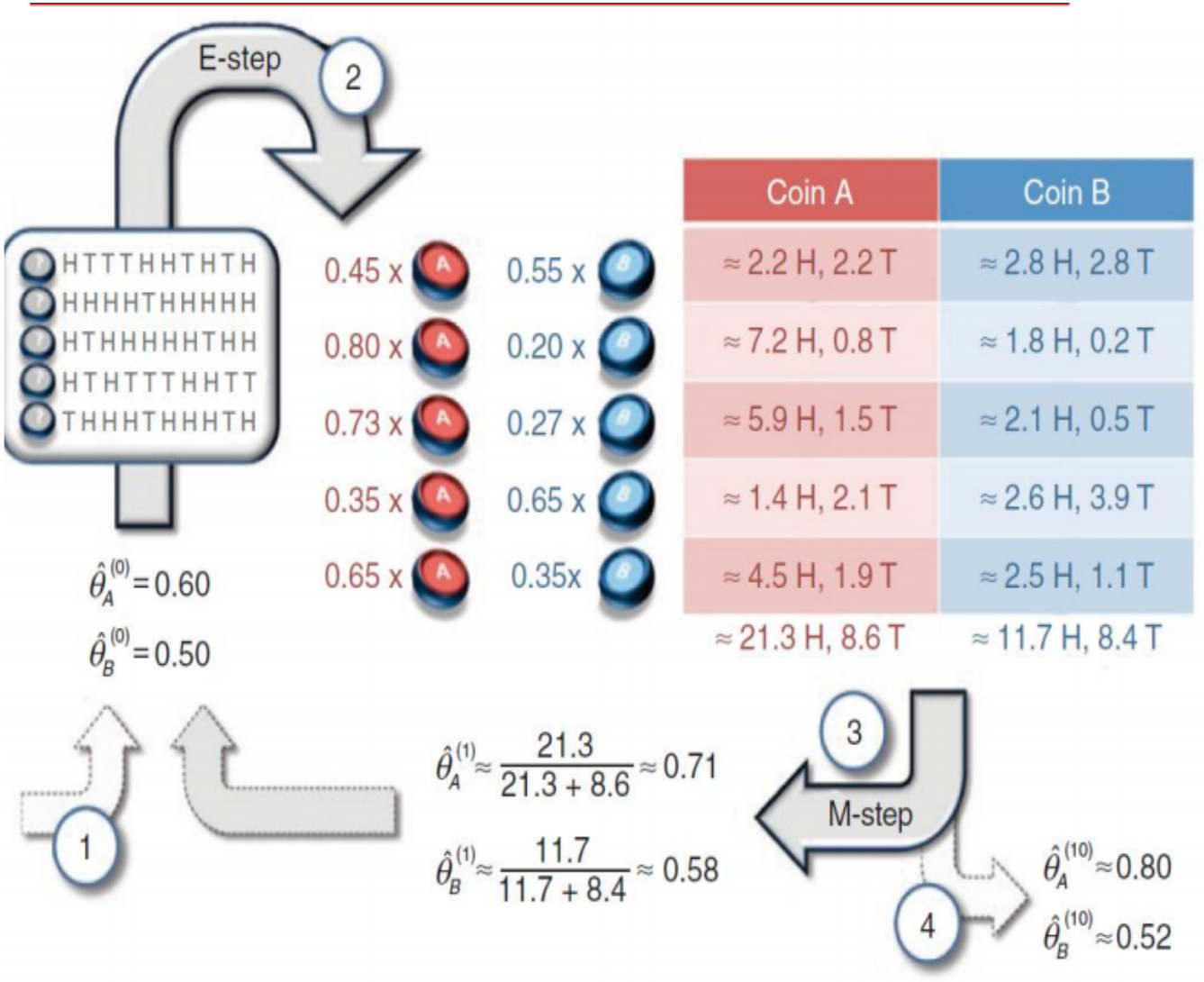
Continued...

Update

$$\theta_A^{(1)} = \frac{w_{1A}X_1 + w_{2A}X_2}{w_{1A}X_1 + w_{2A}X_2 + (10 - X_1)w_{1A} + (10 - X_2)w_{2A}}$$
$$= \frac{0.45 \times 5 + 0.80 \times 9}{0.45 \times 5 + 0.80 \times 9 + 5 \times 0.45 + 1 \times 0.80}$$
$$\approx 0.76.$$

$$\theta_B^{(1)} = \frac{w_{1B}X_1 + w_{2B}X_2}{w_{1B}X_1 + w_{2B}X_2 + (10 - X_1)w_{1B} + (10 - X_2)w_{2B}}$$
$$= \frac{0.55 \times 5 + 0.2 \times 9}{0.55 \times 5 + 0.2 \times 9 + 0.55 \times 5 + 0.2 \times 1}$$
$$\approx 0.61.$$

Continued...



[3] Do, B.C. and Batzoglou, S. (2008). What is the expectation maximization algorithm? Nature Biotechnology, 26, 897–899.

Notations

- $\Theta =$ set of parameters.
- $\theta =$ unknown parameter.
- $X =$ observed data.
- $Z =$ unknown\missing data.
- $f(X, Z|\Theta) =$ complete data density.
- $f(Z|X, \Theta) =$ conditional unobserved data density.
- $f(X|\Theta) =$ marginal observed data density.
- $f(Z|\Theta) =$ marginal unobserved data density.
- $E_{Z|X,\Theta}(g(Z)|x, \Theta) = \int_{\mathcal{Z}} g(z)f(z|x, \Theta)dz$, where $\mathcal{Z}$ denote the domain for the conditional density function $f(Z|X, \Theta)$.

EM Algorithm

- We can define a likelihood function such that

$$L(\Theta|X, Z) = f(X, Z|\Theta).$$

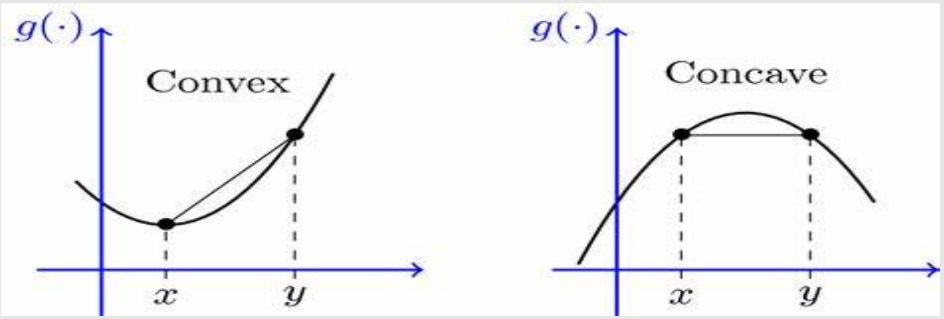
- This function is a random variable since the missing information Z is unknown and random governed by an underlying distribution.
- The original likelihood $L(\Theta|X)$ is referred to as the incomplete-data likelihood function.
- The EM algorithm first finds the expected value of the complete-data log-likelihood $\log f(X, Z|\Theta)$ with respect to the unknown data Z given observed data X and current parameter estimates.

Jensen's Inequality

Definition (Concave Function)

A function g is said to be concave on $\mathbb{R}$ if

$$g(\alpha x + (1-\alpha)y) \geq \alpha g(x) + (1-\alpha)g(y) \quad \text{for all } \alpha \in [0,1].$$



Jensen's Inequality: Let f be a concave function on $\mathbb{R}$ and suppose $\mathbb{E}[X] < \infty$ and $\mathbb{E}[f(X)] < \infty$. Then $f(\mathbb{E}[X]) \geq \mathbb{E}[f(X)]$.

Example

Note that $\log$ is a concave function and hence for a random variable X and function g, we have

EM Algorithm Contd...

For the given data vector X, our goal is to find the ML estimate such that

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}}\, L(\theta|X) = \underset{\theta}{\operatorname{argmax}}\, f(X|\theta) = \underset{\theta}{\operatorname{argmax}} \log f(X|\theta) = l(\theta|X)$$

The key idea of EM algorithm is such as follows:

$$\begin{aligned} l(\theta|X) = \log f(X|\theta) &= \log \int_z f(x,z|\theta)dz = \log \int_z p(z|x,\theta^{(k)}) \frac{f(x,z|\theta)}{p(z|x,\theta^{(k)})} \\ &= \log \mathbb{E}_{Z|X,\theta^{(k)}} \left[\frac{f(x,Z|\theta)}{p(Z|x,\theta^{(k)})} \right] \geq \mathbb{E}_{Z|X,\theta^{(k)}} \left[\log \frac{f(x,Z|\theta)}{p(Z|x,\theta^{(k)})} \right] \\ &= \int_z p(z|x,\theta^{(k)}) \left[\log \frac{f(x,z|\theta)}{p(z|x,\theta^{(k)})} \right] dz \\ &= \int_z p(z|x,\theta^{(k)}) \log f(x,z|\theta)dz - \int_z p(z|x,\theta^{(k)}) \log p(z|x,\theta^{(k)})d \end{aligned}$$

EM Algorithm Contd...

- Thus we have

$$
\begin{aligned}
l(\theta|X) &= \log f(X|\theta) \\
&\geq \int_z p(z|x,\theta^{(k)}) \log f(x,z|\theta) dz - \int_z p(z|x,\theta^{(k)}) \log p(z|x,\theta^{(} \\
&= Q(\theta|\theta^{(k)}) - \int_z p(z|x,\theta^{(k)}) \log p(z|x,\theta^{(k)}) dz.
\end{aligned}
$$

- Rather than maximizing $l(\theta|X)$ the EM algorithm will maximize the lower bound given by

$$
Q(\theta|\theta^{(k)}) - \int_z p(z|x,\theta^{(k)}) \log p(z|x,\theta^{(k)}) dz.
$$

- The term $\int_z p(z|x,\theta^{(k)}) \log p(z|x,\theta^{(k)}) dz$ is independent of θ and hence it will maximize

$$
Q(\theta|\theta^{(k)}) = \mathbb{E}_{Z|X}[\log f(x,Z|\theta)].
$$

EM Algorithm Contd...

- Let $k = 0$. Start with initial estimate for θ as $\theta^{(k)}$.
- Find the conditional density $f(Z|X, \theta^{(k)})$ for the completion variables.
- Calculate the conditional expected log likelihood or "Q"-function:

$$Q(\theta|\theta^{(k)}) = \mathbb{E}[\log f(X, Z|\theta)|X, \theta^{(k)}].$$

  Here, expectation is with respect to the conditional distribution of Z given X and $\theta^{(k)}$.

- Find the θ that maximizes the function $Q(\theta|\theta^{(k)})$ and this new estimate will be $\theta^{(k+1)}$ i.e.

$$\theta^{(k+1)} = \underset{\theta}{\operatorname{argmax}}\, Q(\theta|\theta^{(k)}).$$

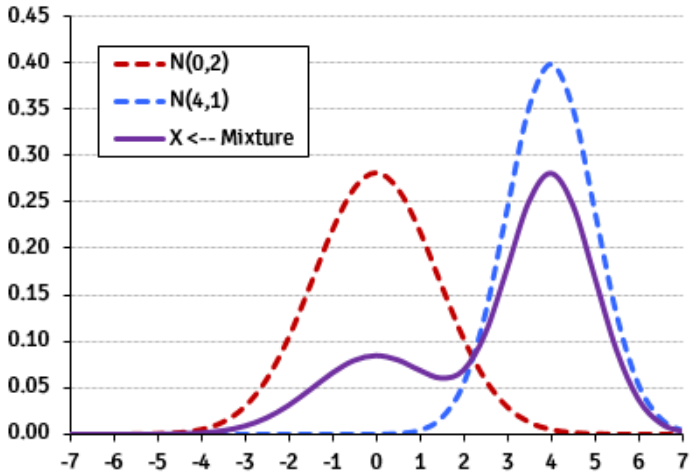
- Let $k := k + 1$ and repeat until convergence; standard criteria for convergence is to iterate until the estimate stops changing i.e. $\|\theta^{(k+1)} - \theta^{(k)}\| < \epsilon$, for the chosen tolerance ϵ.

Mixture distributions

A random vector X is said to arise from a parametric finite mixture distribution if, for all $x \in \text{Supp}(X)$, we can write its density as:

$$f_X(x|\nu) = \sum_{g=1}^{G} \pi_g p_g(x|\theta_g),$$

where $\pi_g > 0$, such that $\sum_{g=1}^{G} \pi_g = 1$, are called mixing proportions, $p_g(x|\theta_g)$ are component densities, and $\nu = (\pi_1, \pi_2, ..., \pi_G, \theta_1, \theta_2, ..., \theta_G)$.



4

[4] Image Source: Internet

EM for Gaussian Mixture Model

- Consider the data $X = \{X_1, X_2, ..., X_n\}$ from Gaussian mixture model with $C = 2$ components. The latent variable for model is $Z_i \in \{1, 2\}$.
- The marginal probability distribution of X_i is of the form $P(X_i = x) = \sum_{c=1}^{2} \pi_c P(X_i = x | Z_i = c)$, where π_c is the mixture proportion representing the probability that X_i belongs to the c-th mixture component.
- The conditional distribution $X_i | Z_i = c \sim N(\mu_c, \sigma_c^2)$.

- E-step: For each data X_i, compute the probability that it belongs to cluster c and denote it by w_{ic}. That is, we guess the values of $Z_i's$ using posterior probability distribution $\mathbb{P}(Z_i = c|X_i)$.

- Set $w_{ic} = \mathbb{P}(Z_i = c|X_i, \mu^{(k)}, (\sigma^2)^{(k)})$,

$$w_{ic} = \frac{\mathbb{P}(X_i|Z_i = c)\mathbb{P}(Z_i = c)}{\sum_{c=1}^{2} \mathbb{P}(X_i|Z_i = c)\mathbb{P}(Z_i = c)}$$
$$= \frac{N(\mu_c^{(k)}, (\sigma_c^2)^{(k)})\pi_c^{(k)}}{\sum_{c=1}^{2} N(\mu_c^{(k)}, (\sigma_c^2))^{(k)}\pi_c^{(k)}}$$

Continued...

- M-step: Now, we use the membership weights w_{ic} and data to update the new parameter values.
- Let $n_c = \sum_{i=1}^{n} w_{ic}$ for each component c.
- Update the parameters as follows:

$$\pi_c^{(k+1)} = \frac{n_c}{n}$$

$$\mu_c^{(k+1)} = \frac{\sum_{i=1}^{n} w_{ic} X_i}{n_c}$$

$$(\sigma_c^2)^{(k+1)} = \frac{\sum_{i=1}^{n} w_{ic} (X_i - \mu_c^{(k+1)})^2}{n_c}.$$

Advantages

- The main advantage of the EM algorithm is that it is easy to implement.
- Its memory requirements tend to be modest.
- It is always guaranteed that likelihood will increase with each iteration and the algorithm will reach a local optima.
- The EM simultaneously optimize a large number of parameters.

Disadvantages

- The main disadvantage of the EM algorithm is its very slow linear convergence in some cases.
- Not guaranteed to get globally optimal estimate, generally converge to local optima.
- In practice multiple local maxima of the likelihood function are frequent and the algorithm converges to a local maxima, the initial estimates can greatly affect the final results.
- The slow linear convergence can be improved by some acceleration sachems but that will increase the complexity of the algorithm.

Example 2: Gaussian Mixture Model (Numeric)

- Data: $x = \{1.0, 1.2, 0.8, 3.0, 3.2, 2.8\}$.
- Model: two Gaussians with equal variance $\sigma^2 = 0.1$, unknown means μ_1, μ_2 and mixing weights π_1, π_2.
- Initialize: $\mu_1^{(0)} = 1$, $\mu_2^{(0)} = 3$, $\pi_1 = \pi_2 = 0.5$.

Gaussian Mixture: E-step (Numeric)

Compute responsibilities for component 1:

$$w_{i1} = \frac{\pi_1 \phi(x_i; \mu_1, \sigma)}{\pi_1 \phi(x_i; \mu_1, \sigma) + \pi_2 \phi(x_i; \mu_2, \sigma)}$$

where $\phi(x; \mu, \sigma)$ is normal pdf.

x_i	w_{i1}	$w_{i2} = 1 - w_{i1}$
1.0	0.99	0.01
1.2	0.99	0.01
0.8	0.99	0.01
3.0	0.01	0.99
3.2	0.01	0.99
2.8	0.01	0.99

Gaussian Mixture: M-step (Numeric)

Update:

$$\pi_1^{new} = \frac{\sum w_{i1}}{6} \approx 0.5, \quad \pi_2^{new} = 1 - \pi_1^{new}.$$

$$\mu_1^{new} = \frac{\sum w_{i1} x_i}{\sum w_{i1}} \approx 1.0, \quad \mu_2^{new} \approx 3.0.$$

- As expected, clusters separate near means 1 and 3.
- Continue iterating until convergence if starting parameters differ more.

Example 3: Poisson Mixture (Count Data)

- Data: counts $x = (2, 3, 4, 0, 1, 5)$.
- Model: two Poisson components with rates λ_1, λ_2, weights π_1, π_2.
- Initialize: $\lambda_1^{(0)} = 1, \lambda_2^{(0)} = 4, \pi_1 = 0.5$.

Poisson Mixture: E-step (Numeric)

$$w_{i1} = \frac{\pi_1 e^{-\lambda_1} \lambda_1^{x_i} / x_i!}{\pi_1 e^{-\lambda_1} \lambda_1^{x_i} / x_i! + \pi_2 e^{-\lambda_2} \lambda_2^{x_i} / x_i!}.$$

x_i	w_{i1}	w_{i2}
2	0.80	0.20
3	0.35	0.65
4	0.10	0.90
0	0.99	0.01
1	0.95	0.05
5	0.05	0.95

Poisson Mixture: M-step (Numeric)

Updated parameters:

$$\pi_1 = \frac{\sum w_{i1}}{6} \approx 0.54, \quad \pi_2 = 0.46.$$

$$\lambda_1 = \frac{\sum w_{i1} x_i}{\sum w_{i1}} \approx 1.2, \quad \lambda_2 \approx 4.2.$$

Iterate until convergence.

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Thank You