CS365 Foundations of Data Science

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 $\Pr(H) = heta_A$



 $\Pr(H) = heta_B$

Process

- Suppose we choose a coin (A or B) uniformly at random (uar)
- We toss the coin n times, and record the total number of heads

We repeat the process k times

- We have two unknown parameters θ_A , θ_B
- Suppose k=5, n=10
- The data are two vectors

 - x=X_H = (x₁, x₂, x₃, x₄, x₅) #heads per round
 z=Z_c = (z₁, z₂, z₃, z₄, z₅) #coin id per round

- E.g.,
$$x=(5,9,8,4,7)$$
, $z=(B,A,A,B,A)$ 3 0

Result seland First coin

(1) coin

(2)

(3)

Comprehension question: What are the MLE for θ_A , θ_B in this case?

$$\begin{array}{c} = O_{A} \cdot (1-\theta_{A}) \cdot O_{B} \cdot (1-\theta_{B}) \\ = O_{A} \cdot (1-\theta_{A}) \cdot O_{A} + O_{A} + O_{A} \cdot (1-\theta_{A}) + O_{A} \cdot O_{B} + O_{A} \cdot O_{A} + O_{A} \cdot O_{A} + O_{A} \cdot O_{A} + O_{A} \cdot O_{A} \cdot O_{A} = O_{A} \cdot O_{A} \cdot O_{A} \cdot O_{A} = O_{A} \cdot O_{A} = O_{A} \cdot O_{$$

Maximum likelihood estimates for the unknown parameters θ_{A} , θ_{B}

Coin A	Coin B	
	5 H, 5 T	
9 H, 1 T		$\hat{\theta}_{A} = \frac{24}{24 + 6}$
8 H, 2 T		â 9
	4 H, 6 T	$\hat{\theta}_{B} = \frac{9}{9+11}$
7 H, 3 T		
24 H, 6 T	9 H, 11 T	

- Suppose we only see the number of heads per round.
 - In other words we do not have access to z
- We refer to z as hidden variables or latent factors
- Remarks
 - 1. Not uncommon/common setting in data science applications ⇒ missing data!
 - 2. Clear that maximizing $Pr(x|\theta)$ is much harder than $Pr(x,z|\theta)$ in the presence of missing data z.

The Expectation-Maximization algorithm

- Also known as the EM algorithm
 - In reality, it is an algorithm design methodology rather than a given algorithm

Maximum Likelihood from Incomplete Data via the EM Algorithm

By A. P. DEMPSTER, N. M. LAIRD and D. B. RUBIN

Harvard University and Educational Testing Service

[Read before the ROYAL STATISTICAL SOCIETY at a meeting organized by the RESEARCH SECTION on Wednesday, December 8th, 1976, Professor S. D. SILVEY in the Chair]

SUMMARY

A broadly applicable algorithm for computing maximum likelihood estimates from incomplete data is presented at various levels of generality. Theory showing the monotone behaviour of the likelihood and convergence of the algorithm is derived. Many examples are sketched, including missing value situations, applications to grouped, censored or truncated data, finite mixture models, variance component estimation, hyperparameter estimation, iteratively reweighted least squares and factor analysis.

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AP Dempster, NM Laird... - Journal of the Royal ..., 1977 - Wiley Online Library

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Let's see the key idea in the context of the two-coins problem before full description

- We will proceed iteratively by updating
- Each iteration starts with a guess of the unknown parameters

$$\hat{ heta}^{(t)} = \left(\hat{ heta}_A^{(t)}, \hat{ heta}_B^{(t)}
ight)$$

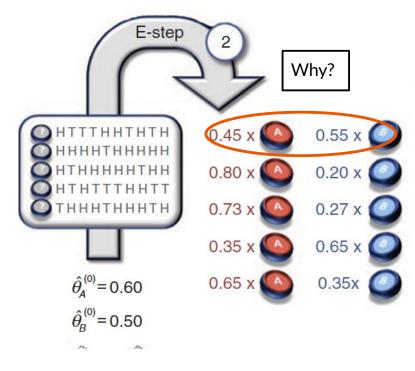
- E-step: a probability distribution over possible completions is computed using the current parameters $\hat{\theta}^{(t)}$
- M-step: the new parameters are determined using the current completions.

Suppose our initial guess for the unknown variables are 0.6, and 0.5.

E-step: what is the probability that round i comes from coin A/coin B?

Coin A:
$$\alpha = 0.6^{\frac{5}{2}} \cdot 0.4^{\frac{5}{2}} \times 0.000796$$

Coin B $\alpha = 0.5^{\frac{5}{2}} \cdot 0.5^{\frac{5}{2}} = \left(\frac{1}{2}\right)^{10} \times 0.000716$
 $P_r(z_1 = A) = \frac{0.6^{\frac{5}{2}} \cdot 0.4^{\frac{5}{2}}}{0.6^{\frac{5}{2}} \cdot 0.4^{\frac{5}{2}} + (0.5)^{10}} = 0.45$, $P_r(z_1 = B) = 0.55$



M-step: In order to learn $\hat{\theta}^{(t+1)} = \left(\hat{\theta}_A^{(t+1)}, \hat{\theta}_B^{(t+1)}\right)$ we first need to estimate

the number of heads/tails from coins A/B given our estimates of the

latent variables.

 Notice that instead of being 100% certain whether a round was due to coin A or B, we have a probability distribution.

Round 1: 5H, 5T

HТТТННТНТН О.45 x О.55 x О.5





	Coin A	Coin B
Heads	0.45x5	0.55x5
Tails	0.45x5	0.55x5

Coin A	Coin B	
≈ 2.2 H, 2.2 T	≈ 2.8 H, 2.8 T	

We repeat this for all five rounds

One more round

Round 2: 9H, 1T From the E-round we have





Coin B or
$$0.5^9$$
 $0.5^4 = \left(\frac{1}{2}\right)^{10} \times 0.000936$

$$P_{r}\left(\frac{2}{2}=A\right) = \frac{0.6^{9} \cdot 0.4^{\frac{1}{2}}}{0.6^{9} \cdot 0.4^{\frac{1}{2}} + (0.5)^{10}} = 0.8041 \times 0.8, P_{r}\left(\frac{2}{2}=3\right) = 0.2$$

	Coin A	Coin B
Heads	0.8x9	0.2x9
Tails	0.8x1	0.2x1

≈ 7.2 H, 0.8 T

≈ 1.8 H, 0.2 T

- Having done this for all 5 rounds we obtain the following

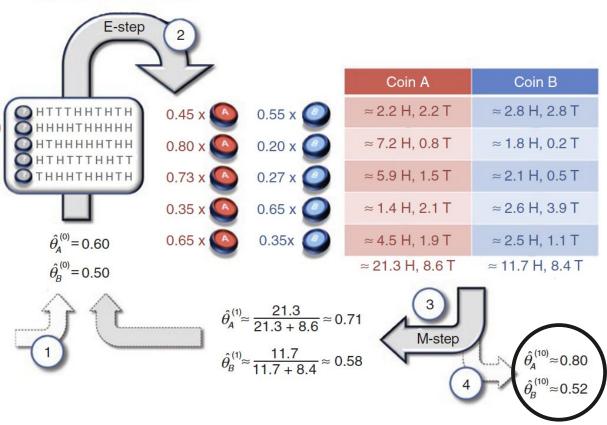
Coin A	Coin B	
≈ 2.2 H, 2.2 T	≈ 2.8 H, 2.8 T	
≈ 7.2 H, 0.8 T	≈ 1.8 H, 0.2 T	
≈ 5.9 H, 1.5 T	≈ 2.1 H, 0.5 T	
≈ 1.4 H, 2.1 T	≈ 2.6 H, 3.9 T	
≈ 4.5 H, 1.9 T	≈ 2.5 H, 1.1 T	
≈213H 86T	≈117H84T	

- The M-step now simply becomes the MLEs according to this data

$$\hat{\theta}_{A}^{(1)} \approx \frac{21.3}{21.3 + 8.6} \approx 0.71$$

$$\hat{\theta}_{B}^{(1)} \approx \frac{11.7}{11.7 + 8.4} \approx 0.58$$





EM algorithm

- Suppose maximizing $Pr(x|\theta)$ has no closed form solution/intractable.
- Key idea: latent variables z that make likelihood computations tractable
- Intuition: $Pr(x,z|\theta)$, $Pr(z|x,\theta)$ should be easy to compute after introducing the "right" latent variables.
- EM guaranteed to converge to a local maximum!

EM algorithm

Define the "expected log" $Q(\theta|\theta')$ where θ' is the current estimate of θ :

$$Qig(heta \mid heta'ig) = \sum_{z} \Prig(z \mid x, heta'ig) \log \Pr(x, z \mid heta)$$

The EM algorithm is an iterative method consisting of two steps.

- 1. E-step: Find $Q(\theta|\theta')$ in terms of the latent variables z
- 2. M-step: Find θ^* maximizing Q($\theta | \theta'$)

EM-algorithm

Some remarks

- 1. The quantity Q typically is not computed, but is useful for proving the convergence of the EM algorithm.
- 2. What we really need to know is the distribution of z given x, our guess θ , and frequently knowing the expectation of z over its distribution suffices as we saw in our example.
- 3. The M-step maximizes Q over all possible θ values. Ideally, knowing x and z allows an easy maximization over θ .

Readings

- 1. What is the EM algorithm?
- 2. Wikipedia article
- 3. Original EM paper
- 4. Andrew Ng's notes

