Expectation Maximisation (EM)

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Outline ... EM

- Importance
- Goal
- Idea
- Derivation
- Visualisation

Importance ...

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



Dempster, A. P., Laird, N. M. & Rubin, D. B. (1977). *Maximum likelihood from incomplete data via the EM algorithm*. **Journal of the Royal Statistical Society**: Series B, 39, 1-38.

Importance ...

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by AP Dempster · 1977 · Cited by 69463 — A broadly applicable algorithm for computing maximum likelihood estimates from incomplete data is presented at various levels of generality.

21, Feb, 2023



Importance ...

Keywords ...

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Setup

$$X:observable rv^*$$

$$\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N\},$$

$$\mathbf{x}_i \in \mathbb{R}^{D_1}$$

$$X: observable ext{ rv}^*$$
 $Z: latent ext{ rv}$ $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N\}, \quad \mathbf{x}_i \in \mathbb{R}^{D_1}$ $\mathbf{Z} = \{\mathbf{z}_1, \mathbf{z}_2, ..., \mathbf{z}_N\}, \quad \mathbf{z}_i \in \mathbb{R}^{D_2}$

 $\mathbf{X}: incomplete \ \mathrm{data}$

 $\{\mathbf{X}, \mathbf{Z}\}$: complete data

 θ : model parameters

Setup

independent

$$p(\mathbf{X}|\theta) = p(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N|\theta)$$
 identically distributed
$$p(\mathbf{X}|\theta) = \sum_{i=1}^{N} \log p(\mathbf{x}_i|\theta)$$
 $p(\mathbf{x}_i|\theta)$

$$p(\mathbf{X}, \mathbf{Z}|\theta) = p(\mathbf{x}_1, \mathbf{z}_1, \mathbf{x}_2, \mathbf{z}_2, ..., \mathbf{x}_N, \mathbf{z}_N | \theta) \stackrel{i.i.d}{=} \prod_{i=1}^{N} p(\mathbf{x}_i, \mathbf{z}_i | \theta)$$
$$\log p(\mathbf{X}|\theta) = \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\theta)$$

Setup

$$P(\mathbf{X}|\theta)$$
: incomplete data likelihood

$$P(\mathbf{X}, \mathbf{Z}|\theta)$$
: complete data likelihood

$$P(\mathbf{Z}|\mathbf{X}, \theta) : posterior \text{ probability}$$

Marginalisation

$$p(\mathbf{X}|\theta) = \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\theta)$$

Chain rule (probability)

$$p(\mathbf{X}|\theta) = \frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{p(\mathbf{Z}|\mathbf{X}, \theta)}$$

Goal ...

$$\theta_{ML}^* = \underset{\theta \in \Theta}{\operatorname{argmax}} \ p(\mathbf{X}|\theta) = \underset{\theta \in \Theta}{\operatorname{argmax}} \ \log p(\mathbf{X}|\theta)$$

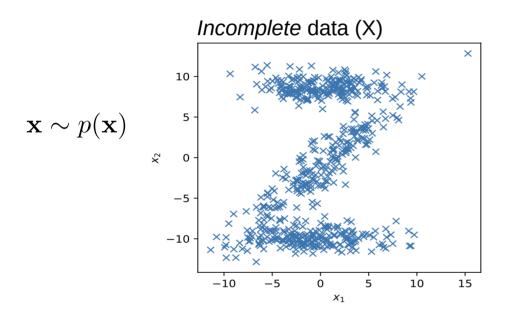
- log is *strictly increasing* → argmax remains identical
- Advantages:
 - ✓ Mathematical convenience → log[exp(.)]
 - Numerical Stability

Goal ...

$$\theta_{ML}^*(\mathbf{X}|\theta) = \underset{\theta \in \Theta}{\operatorname{argmax}} \log p(\mathbf{X}|\theta)$$
$$= \underset{\theta \in \Theta}{\operatorname{argmax}} \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\theta)$$

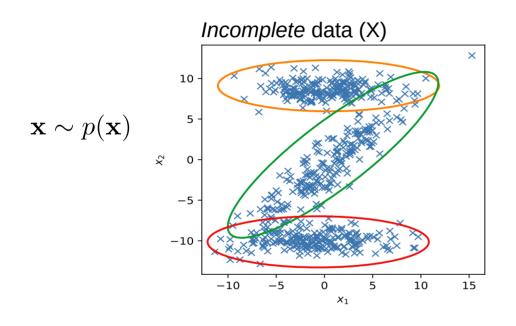
EM assumes model includes *latent variables* (**Z**).

Latent Variable (Z)



Interpretation: *latent variable* is a part of a model ... *explains* **X**.

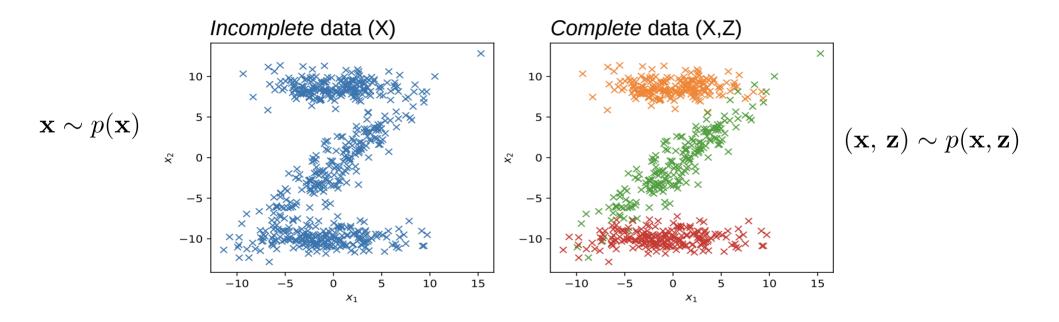
Latent Variable (Z)



Consider clustering ...

Interpretation: *latent variable* is a part of a model ... *explains* **X**.

Latent Variable (Z)



Interpretation: *latent variable* is a part of a model ... *explains X*.

Direct Solution

$$\theta_{ML}^* = \underset{\theta \in \Theta}{\operatorname{argmax}} \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} | \theta)$$

$$\log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} | \theta)$$

$$\frac{\partial \log p(\mathbf{X}|\theta)}{\partial \theta} = 0$$

Step 1

Step 2

$$\left. \frac{\partial^2 \log p(\mathbf{X}|\theta)}{\partial \theta^2} \right|_{\theta = \theta_0} < 0$$

Step 3



 θ_0 : derivative roots

Direct Solution

$$\theta_{ML}^* = \underset{\theta \in \Theta}{\operatorname{argmax}} \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} | \theta)$$

$$\log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} | \theta)$$

Intractable (no closed-form solution)

$$\frac{\partial \log p(\mathbf{X}|\theta)}{\partial \theta} = 0$$

Step 1

Step 2

$$\left. \frac{\partial^2 \log p(\mathbf{X}|\theta)}{\partial \theta^2} \right|_{\theta = \theta_0} < 0$$

Step 3

 θ_0 : derivative roots

Direction solution does not work!

$$\log \sum_{z} p(x,z|\theta) = \log(\ldots + w_{z_i}e^{\frac{(x-\mu_i)^2}{2\sigma_i^2}} + \ldots + w_{z_j}e^{\frac{(x-\mu_j)^2}{2\sigma_j^2}} + \ldots)$$
 Consider simplest case ... Gaussian

$$\frac{\partial \log p(x|\theta)}{\partial \theta} = 0$$

Intractable

Direction solution does not work!

$$\log \sum p(x, z | \theta) = \log(\dots + w_{z_i} e^{\frac{(x - \mu_i)^2}{2\sigma_i^2}} + \dots + w_{z_j} e^{\frac{(x - \mu_j)^2}{2\sigma_j^2}} + \dots)$$

 $\dots = 0 \rightarrow Intractable$

Direction solution does not work!

$$\log \sum_{z} p(x,z|\theta) = \log(... + w_{z_i}e^{\frac{(x-\mu_i)^2}{2\sigma_i^2}} + ... + w_{z_j}e^{\frac{(x-\mu_j)^2}{2\sigma_j^2}} + ...)$$
 ... = 0 \rightarrow Intractable if we could swap $\log \& \Sigma$ = 0 \rightarrow Tractable
$$\sum_{z} \log p(x,z|\theta) = (... + w_i \log e^{\frac{(x-\mu_i)^2}{2\sigma_i^2}} + ... + w_j \log e^{\frac{(x-\mu_j)^2}{2\sigma_j^2}} + ...)$$

$$= (... + c_i(x-\mu_i)^2 + ... + c_j(x-\mu_j)^2 + ...)$$

Optimise ... θ^*

$$\log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} | \theta)$$



Optimise ... θ^*

$$\sum_{\mathbf{Z}} \log p(\mathbf{X}, \mathbf{Z} | \theta)$$

Intractable

Tractable



$$\log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} | \theta)$$



Optimise ... θ^*

$$\sum_{\mathbf{Z}} \log p(\mathbf{X}, \mathbf{Z} | \theta)$$

Intractable

Tractable

Your problem is to bridge the gap which exists between where you are now and the goal you intend to reach.

Earl Nightingale (1921-1989)

Optimise ... θ^*

$$\log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} | \theta)$$



Optimise ... θ*

$$\sum_{\mathbf{Z}} \log p(\mathbf{X}, \mathbf{Z} | \theta)$$

Intractable

Tractable

Your problem is to bridge the gap which exists between where you are now and the goal you intend to reach.

Earl Nightingale (1921-1989)

$$p(\mathbf{X}|\theta) = \frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{p(\mathbf{Z}|\mathbf{X}, \theta)}$$

Step 0: write $p(X|\theta)$ using *chain rule*

$$p(\mathbf{X}|\theta) = \frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{p(\mathbf{Z}|\mathbf{X}, \theta)} \frac{q(\mathbf{Z})}{q(\mathbf{Z})}$$

$$= \frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} \frac{q(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{X}, \theta)}$$

Step 1: Multiply right-hand side in a *special 1*

$$\log p(\mathbf{X}|\theta) = \log \left[\frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} \frac{q(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{X}, \theta)} \right]$$
$$= \log \left[\frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} \right] + \log \left[\frac{q(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{X}, \theta)} \right]$$

Step 2: Take *log* from both sides

$$q(\mathbf{Z})\log p(\mathbf{X}|\theta) = q(\mathbf{Z})\log \left\lfloor \frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} \right\rfloor + q(\mathbf{Z})\log \left\lfloor \frac{q(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{X}, \theta)} \right\rfloor$$

Step 3: Multiply both sides by q(Z)

$$\sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X}|\theta) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} \right] + \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{q(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{X}, \theta)} \right]$$

Step 4: *Marginalise* over **Z**

$$\sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X}|\theta) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} \right] + \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{q(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{X}, \theta)} \right]$$

$$\log p(\mathbf{X}|\theta) = \dots$$

Step 4: *Marginalise* over *Z*

$$\log p(\mathbf{X}|\theta) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} \right] + \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{q(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{X}, \theta)} \right]$$

$$\log p(\mathbf{X}|\theta) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} \right] + \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{q(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{X}, \theta)} \right]$$

$$\log p(\mathbf{X}|\theta) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} \right] + \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{q(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{X}, \theta)} \right]$$

$$D_{KL}(q \mid\mid p) \triangleq \sum_{y} q(y) \log \frac{q(y)}{p(y)}$$

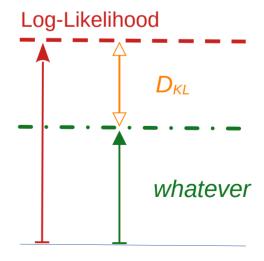
- *D_{KL}* (*KL Divergence*) properties:
 - $\sim D_{KL}(q || p) \ge 0$
 - $VD_{KL}(q || p) = 0 \stackrel{\text{iff}}{\leftrightarrow} q = p$

$$\log p(\mathbf{X}|\theta) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} \right] + \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{q(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{X}, \theta)} \right]$$

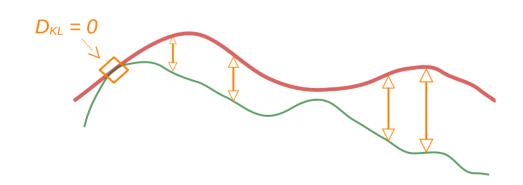
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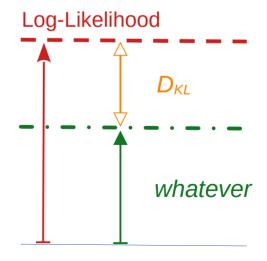
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$$\log p(\mathbf{X}|\theta) = \text{whatever} + \underbrace{D_{KL}(q(\mathbf{Z}) \mid\mid p(\mathbf{Z}|\mathbf{X}, \theta))}_{\geq 0}$$



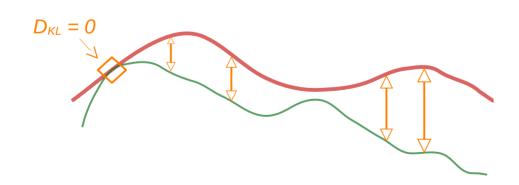
$$\log p(\mathbf{X}|\theta) = \text{whatever} + \underbrace{D_{KL}(q(\mathbf{Z}) \mid\mid p(\mathbf{Z}|\mathbf{X}, \theta))}_{\geq 0}$$

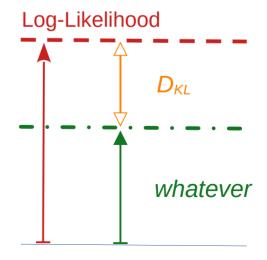




$$\log p(\mathbf{X}|\theta) = \text{whatever} + \underbrace{D_{KL}(q(\mathbf{Z}) \mid\mid p(\mathbf{Z}|\mathbf{X}, \theta))}_{\geq 0}$$

$$\log p(\mathbf{X}|\theta) \geq \text{whatever}$$



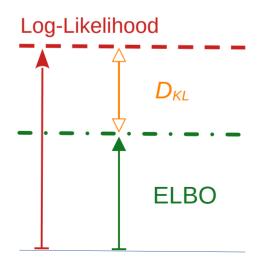


$$\log p(\mathbf{X}|\theta) = \text{ELBO} + \underbrace{D_{KL}(q(\mathbf{Z}) \mid\mid p(\mathbf{Z}|\mathbf{X}, \theta))}_{\geq 0}$$

$$\log p(\mathbf{X}|\theta) \geq \text{ELBO}$$

Evidence Lower Bound (ELBO)

Evidence ≡ log-likelihood



$$\log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{p(\mathbf{X}, \mathbf{Z} | \theta)}{q(\mathbf{Z})} \right] + \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{q(\mathbf{Z})}{p(\mathbf{Z} | \mathbf{X}, \theta)} \right]$$

$$ELBO(q, \theta)$$

$$ELBO(q, \theta)$$

E. Loweimi 20/32

EM Derivation – Step 6

$$\log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{p(\mathbf{X}, \mathbf{Z} | \theta)}{q(\mathbf{Z})} \right] + \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{q(\mathbf{Z})}{p(\mathbf{Z} | \mathbf{X}, \theta)} \right]$$

$$ELBO(q, \theta)$$

$$ELBO(q, \theta)$$

$$\theta_{ML}^* = \underset{\theta \in \Theta}{\operatorname{argmax}} \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} | \theta)$$

Direction solution does not work!

$$\log \sum_{z} p(x,z|\theta) = \log(... + w_{z_i}e^{\frac{(x-\mu_i)^2}{2\sigma_i^2}} + ... + w_{z_j}e^{\frac{(x-\mu_j)^2}{2\sigma_j^2}} + ...)$$

$$... = 0 \rightarrow \text{Intractable}$$

$$\sum_{z} \log p(x,z|\theta) = (... + w_i \log e^{\frac{(x-\mu_i)^2}{2\sigma_i^2}} + ... + w_j \log e^{\frac{(x-\mu_j)^2}{2\sigma_j^2}} + ...)$$

$$= (... + c_i(x-\mu_i)^2 + ... + c_j(x-\mu_j)^2 + ...)$$

EM Derivation – Step 5

$$\underbrace{\log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z})}_{\log p(\mathbf{X}|\theta)} = \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} \right]}_{ELBO(q,\theta)} + \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{q(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{X}, \theta)} \right]}_{D_{KL}(q,\theta)}$$

Intractable!

 $\log \sum p(\mathbf{X}, \mathbf{Z}|\theta)$



$$\sum_{\mathbf{Z}} \log p(\mathbf{X}, \mathbf{Z} | \theta)$$

EM Derivation – Step 6

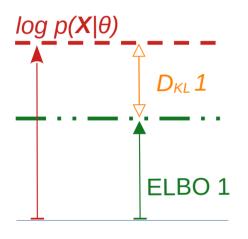
$$\frac{\log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z})}{\log p(\mathbf{X}|\theta)} = \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} \right]}_{ELBO(q,\theta)} + \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{q(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{X}, \theta)} \right]}_{D_{KL}(q,\theta)}$$

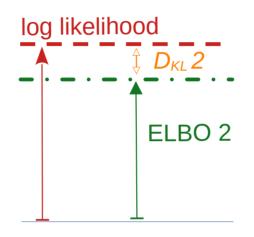
$$\theta^* = \underset{\theta \in \Theta}{\operatorname{argmax}} ELBO$$

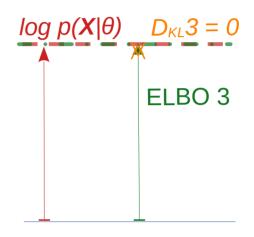


EM → Instead of log-likelihood ... maximise ELBO ...

Best ELBO to optimise ...

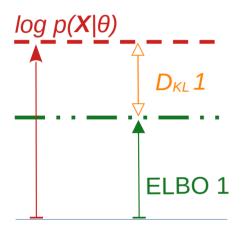


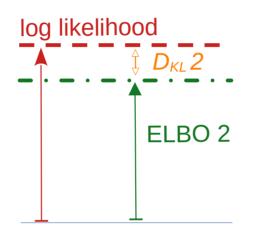


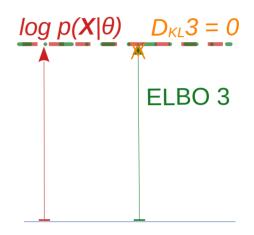


Which ELBO is better?

Best ELBO to optimise ...

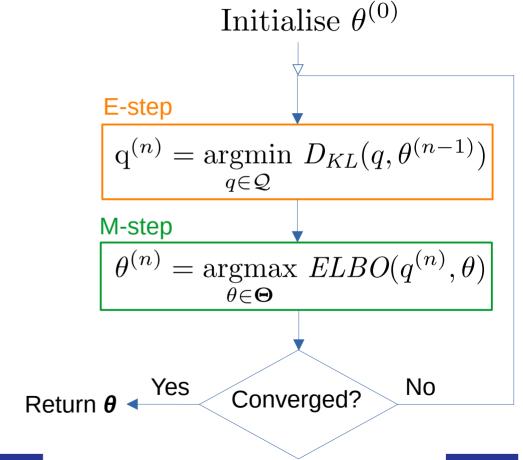






- Lower $D_{KL} \rightarrow \text{Better ELBO (closer to } log p(X|\theta))$
- IDEAL: $D_{KL} = 0 \rightarrow \text{Best ELBO} = \log p(X|\theta)$

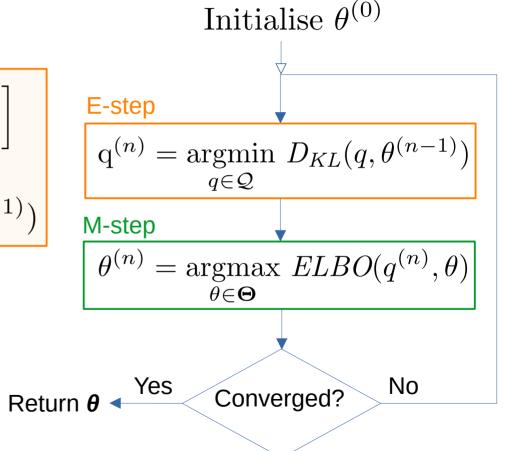
EM Procedure



E-Step

$$D_{KL}(q, \theta^{(n-1)}) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{q(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{X}, \theta^{(n-1)})} \right]$$

$$\operatorname{Min} D_{KL} = 0 \leftrightarrow q^{(n)}(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \theta^{(n-1)})$$



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25/32

M-Step

$$ELBO(q^{(n)}, \theta) = \sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log \left[\frac{p(\mathbf{X}, \mathbf{Z} | \theta)}{q^{(n)}(\mathbf{Z})} \right]$$
$$= \sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z} | \theta) - \sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log q^{(n)}(\mathbf{Z})$$
constant

M-Step

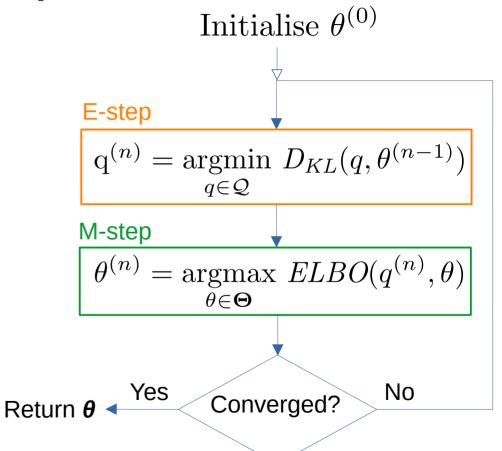
$$ELBO(q^{(n)}, \theta) = \sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log \left[\frac{p(\mathbf{X}, \mathbf{Z} | \theta)}{q^{(n)}(\mathbf{Z})} \right]$$
$$= \sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z} | \theta) - \sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log q^{(n)}(\mathbf{Z})$$
constant

$$\theta^* = \underset{\theta \in \Theta}{\operatorname{argmax}} ELBO(q^{(n)}, \theta)$$
$$= \underset{\theta \in \Theta}{\operatorname{argmax}} \sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z} | \theta)$$

M-Step

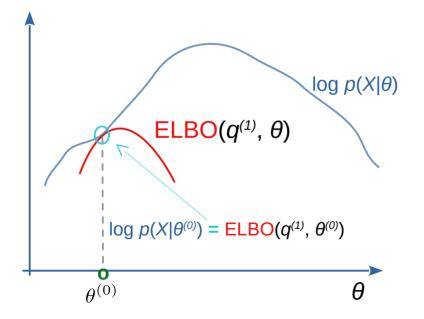
M-step

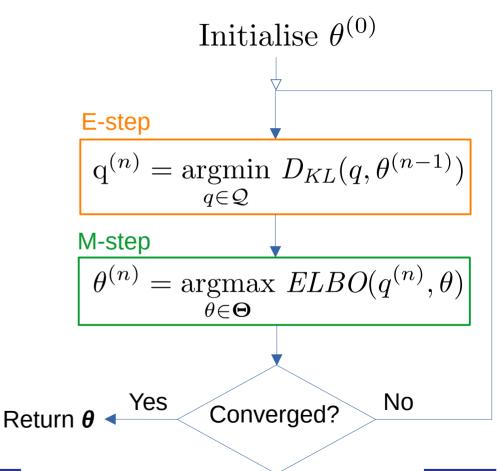
$$\theta^* = \underset{\theta \in \Theta}{\operatorname{argmax}} ELBO(q^{(n)}, \theta)$$
$$= \underset{\theta \in \Theta}{\operatorname{argmax}} \sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z} | \theta)$$



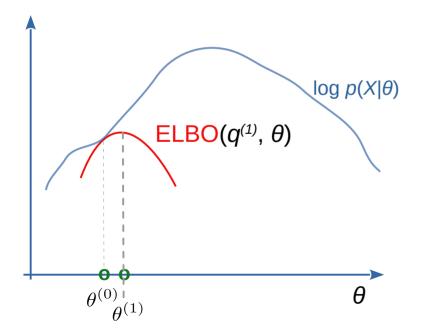
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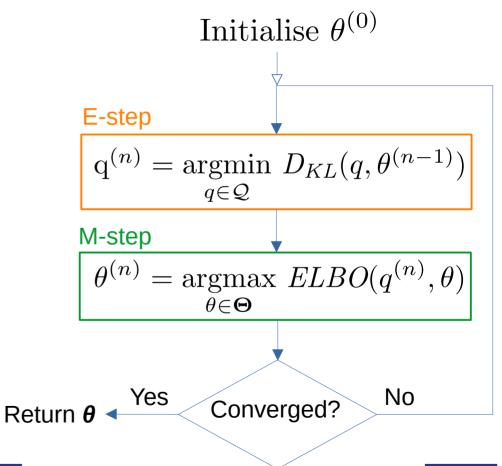
E-step: $q^{(1)}$ = argmin $D_{KL}(q, \theta^{(0)})$

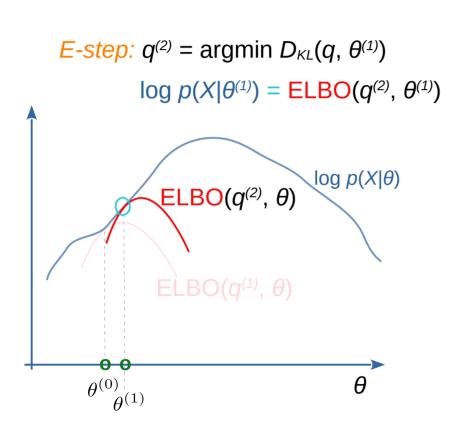




M-step: $\theta^{(1)} = \operatorname{argmax} ELBO(q^{(1)}, \theta)$

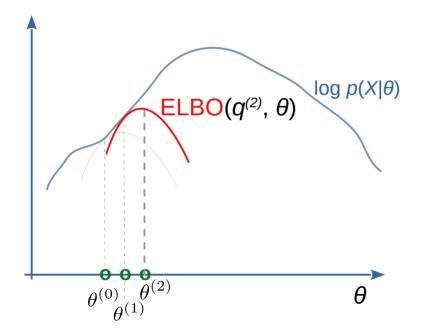






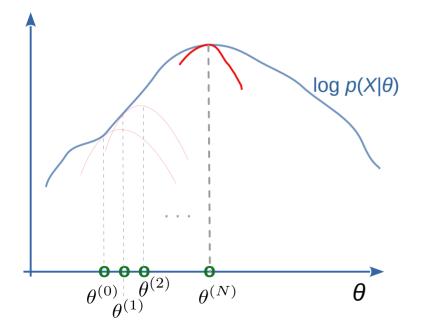


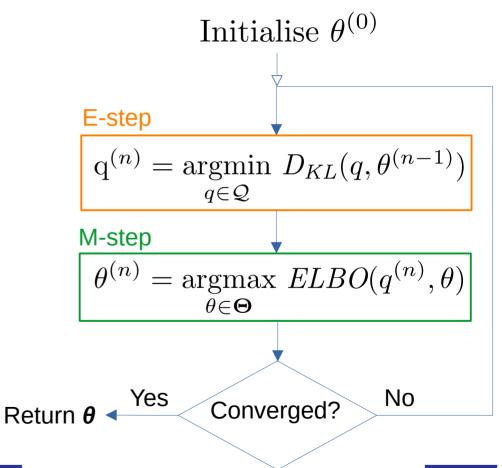
M-step: $\theta^{(2)} = \operatorname{argmax} ELBO(q^{(2)}, \theta)$



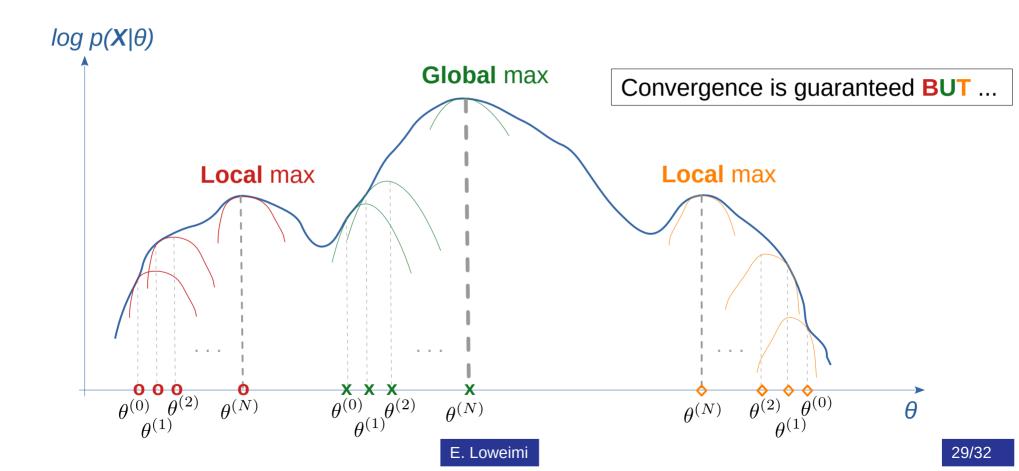


M-step: $\theta^{(N)} = \operatorname{argmax} ELBO(q^{(N)}, \theta)$



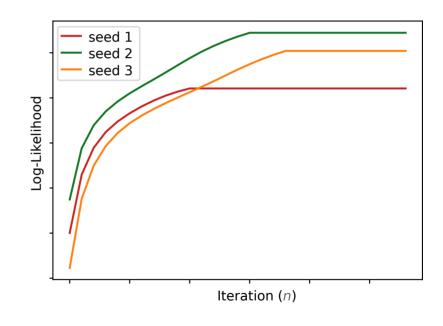


Initialisation Matters (1)



Initialisation Matters (2)

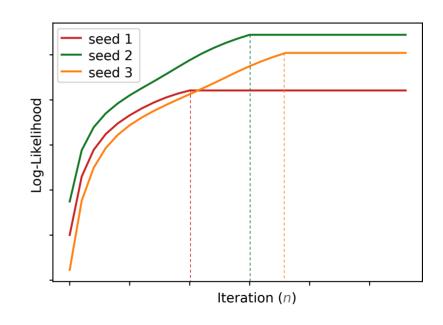
- $p(X|\theta^{(n)})$ is **ALWAYS** non-decreasing
 - $\checkmark ELBO*(q^{(n+1)}, \theta^{(n+1)}) \ge ELBO*(q^{(n)}, \theta^{(n)})$
 - Convergence is guaranteed ... but to local optimum ...



Initialisation Matters (3)

• $p(X|\theta^{(n)})$ is **ALWAYS** non-decreasing

 Initialisation affects ... convergence rate and final log-likelihood

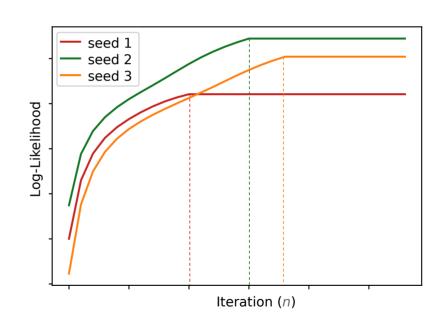


Initialisation Matters (3)

• $p(X|\theta^{(n)})$ is **ALWAYS** non-decreasing

 Initialisation affects ... convergence rate and final log-likelihood

Try multiple initialisations and pick up the best local optimum (highest log-likelihood).



Other Considerations

- EM is closely related to Coordinate Ascent [App B]
 - E-step: fix θ , optimise q
 - M-step: fix \mathbf{q} , optimise θ
- EM shines when M-step can be solved analytically
- Alternatives when M-step is intractable ...
 - Generalised EM (GEM) → (conjugate) gradient ascent in M-Step
 - Expectation Conditional Maximisation (ECM) → coordinate ascent in M-step

Wrap-up ... EM ...

- Goal: estimate θ_{ML} for probabilistic models with latent var
- **How**: an iterative two-stage (E-step, M-step) procedure
- Applications: GMM, HMM, Computational biology, ...
- **Assignment**: estimate θ_{MAP} using EM
- Appendices
 - (A) Further Reading
 - (B) Coordinate Ascent



(A) Further Reading

- Murphy, Chapter 8, Section 7.2, Pages 306-310
- Bishop, Chapter 9, Section 4, Pages 450-455
- Andrew Ng's Lecture Notes, Chapter 11, Pages 142-147

Useful blogs: Link 1 Link 2

(B) Coordinate Ascent

- Iterative optimisation method for multi-variate functions f(x)
- **Idea**: Maximise over <u>one</u> variable (or a block of variables) at a time, assuming others are constants

```
Procedure:

INITIALISE \mathbf{x}^{(0)} = [x_0, x_1, ..., x_{D-1}]

FOR i in range(#iterations):

FOR d in range(D):

\mathbf{x}^{(i)}[d] \leftarrow \operatorname{argmax} f(\mathbf{x}^{(i)}[:d], x_d, \mathbf{x}^{(i-1)}[d+1:])

X_d
```

