Expectation Maximisation (EM)

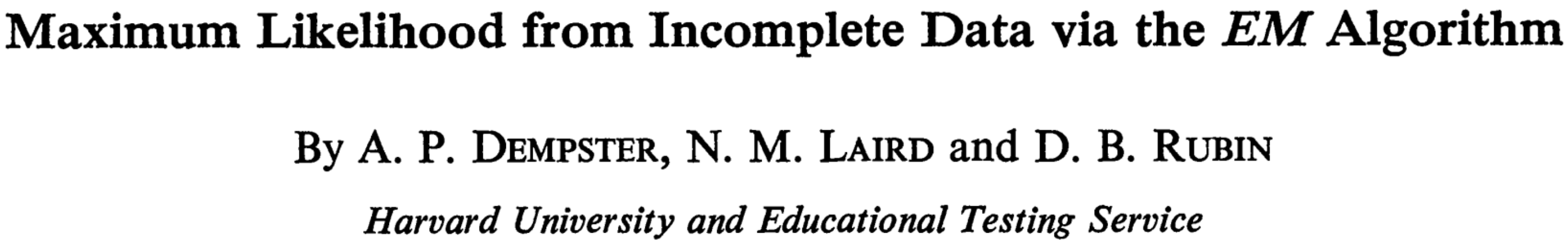
Erfan Loweimi

Speech Group, Machine Intelligence Lab, University of Cambridge

Outline … EM

- Importance
- Goal
- Idea
- Derivation
- Visualisation

Importance ...



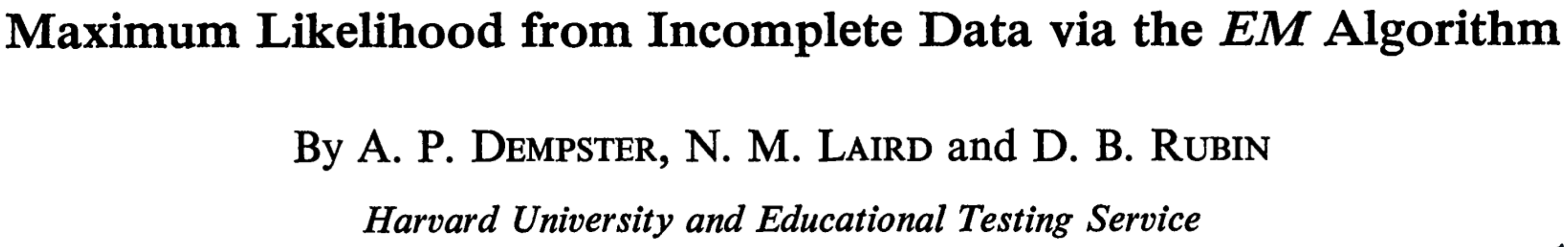
Maximum Likelihood from Incomplete Data via the *EM* Algorithm

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.

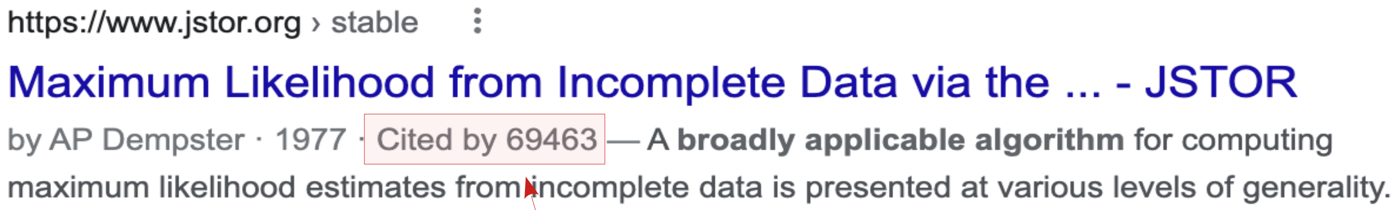
Importance ...



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



https://www.jstor.org › stable

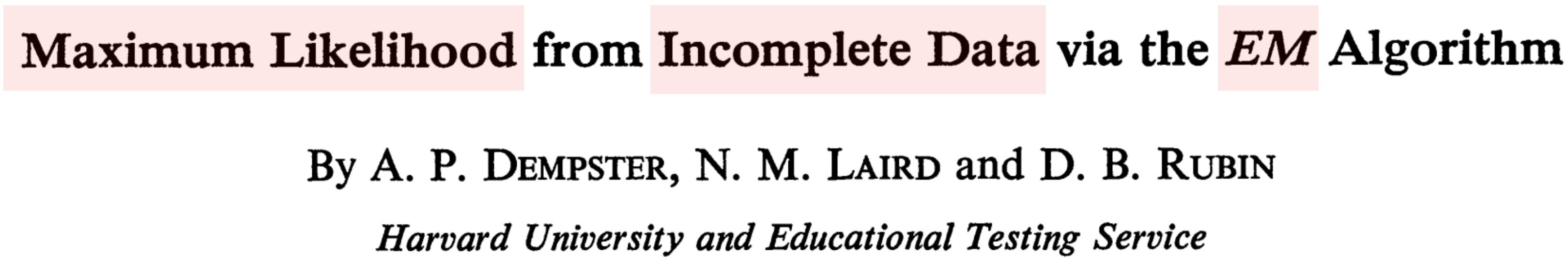
Maximum Likelihood from Incomplete Data via the ... - JSTOR

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 ...



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

https://www.jstor.org › stable

Maximum Likelihood from Incomplete Data via the ... - JSTOR

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

Setup

X : *observable* rv*

$$\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N\}, \quad \mathbf{x}_i \in \mathbb{R}^{D_1}$$

Z : *latent* rv

$$\mathbf{Z} = \{\mathbf{z}_1, \mathbf{z}_2, ..., \mathbf{z}_N\}, \quad \mathbf{z}_i \in \mathbb{R}^{D_2}$$

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

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

θ : model parameters

* rv: random variable

Setup

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

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

$P(\mathbf{Z}|\mathbf{X},\theta)$: *posterior* 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 ...

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

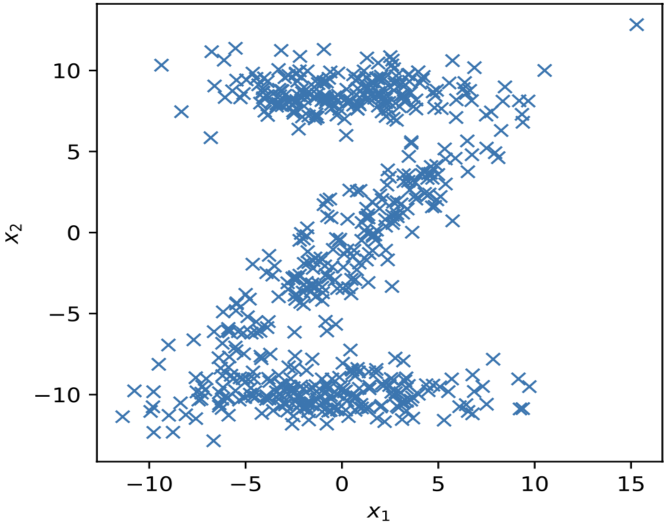
$$= \underset{\theta\in\Theta}{\text{argmax}}\ \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\theta)$$

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

Latent Variable (Z)

$$\mathbf{x} \sim p(\mathbf{x})$$

Incomplete data (X)

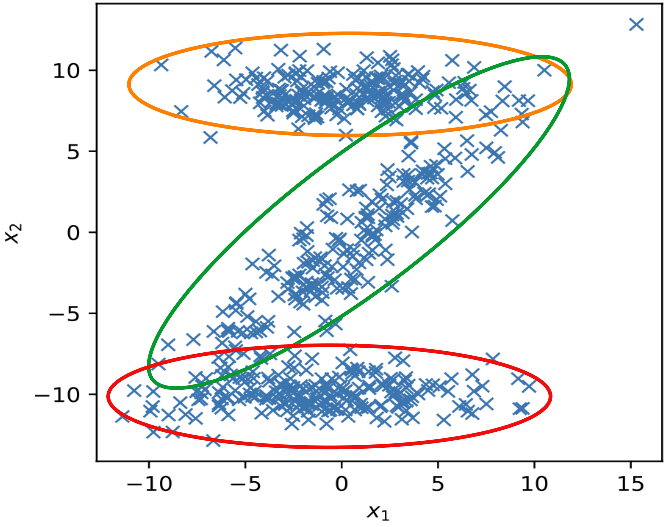


Interpretation: *latent variable* is a part of model ... to explain ***X***.

Latent Variable (Z)

$$\mathbf{x} \sim p(\mathbf{x})$$

Incomplete data (X)



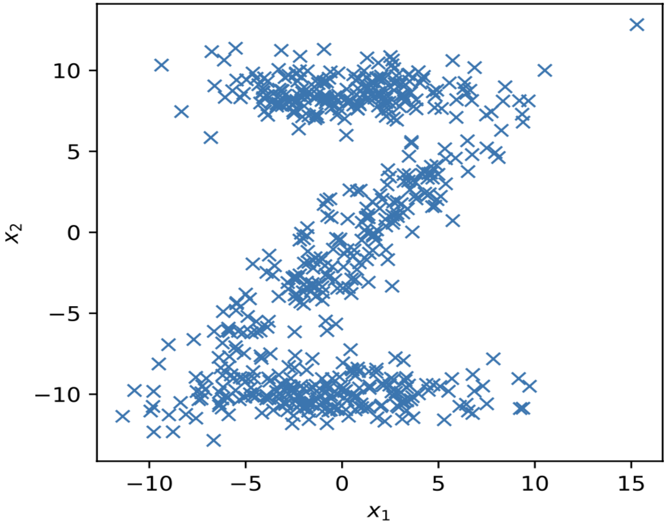
Consider clustering ...

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

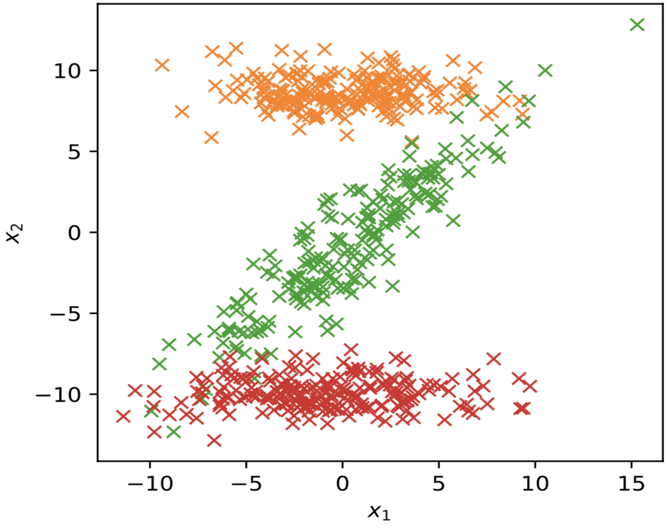
Latent Variable (Z)

$$\mathbf{x} \sim p(\mathbf{x})$$

Incomplete data (X)



Complete data (X,Z)



$$(\mathbf{x},\ \mathbf{z}) \sim p(\mathbf{x}, \mathbf{z})$$

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

Direct Solution

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

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

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

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

Intractable (no closed-form solution)

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

Step 1

Step 2

Step 3

θ_0: derivative roots

Direction solution does not work!

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

Consider simplest case ... Gaussian

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

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 → Intractable

Direction solution does not work!

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

… = 0 → Intractable

If we could swap log & Σ ...

… = 0 → Tractable

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

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

Optimise … θ^*

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

Intractable

≠

Optimise … θ^*

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

Tractable

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)

EM

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)

EM Derivation – Step 0

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

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

EM Derivation – Step 1

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

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

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

EM Derivation – Step 2

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

Step 2: Take *log* from both sides

EM Derivation – Step 3

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

Step 3: Multiply both sides by *q(Z)*

EM Derivation – Step 4

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

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

EM Derivation – Step 4

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

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

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

EM Derivation – Step 5

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

EM Derivation – Step 5.1

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

EM Derivation – Step 5.1

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

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

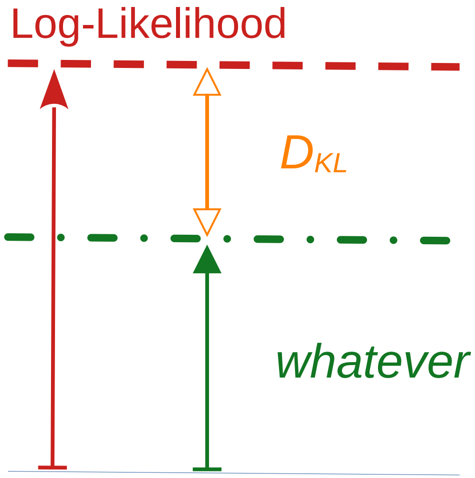
- *D_{KL} (KL Divergence)* properties:
  - ✓ $D_{KL}(q \mid\mid p) \geq 0$
  - ✓ $D_{KL}(q \mid\mid p) = 0 \leftrightarrow q = p$

EM Derivation – Step 5.2

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

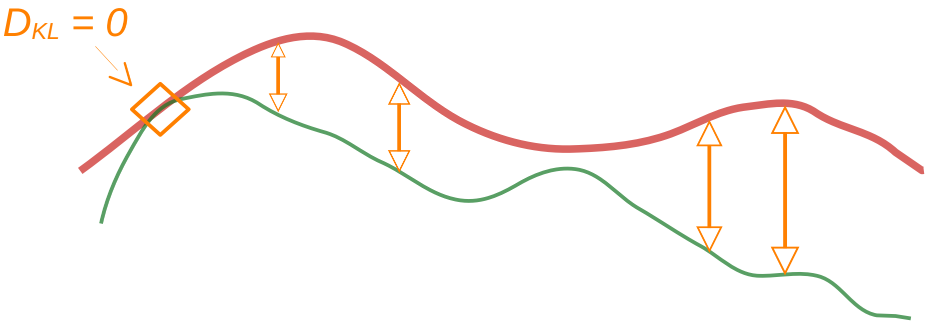
EM Derivation – Step 5.2

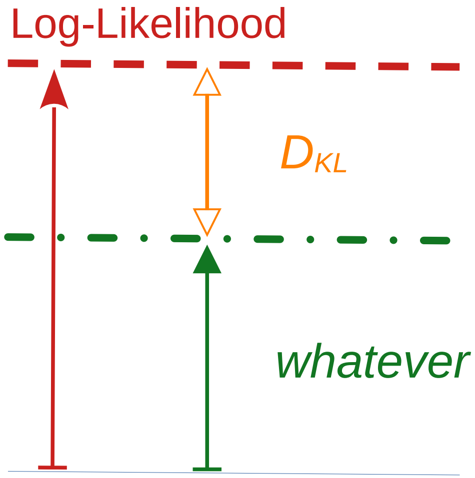
$$\log p(\mathbf{X}|\theta) = \text{whatever} + \underbrace{D_{KL}(q(\mathbf{Z}) \mid\mid p(\mathbf{Z}|\mathbf{X}, \theta))}_{\geq 0}$$



EM Derivation – Step 5.2

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

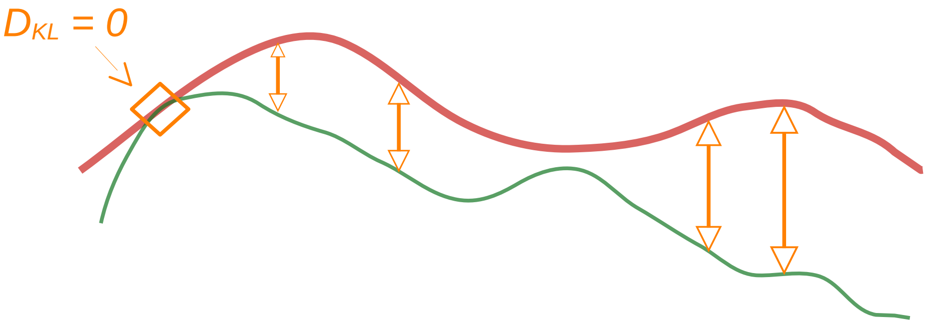


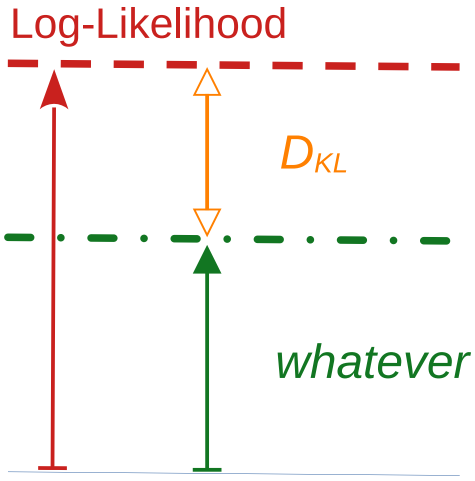


EM Derivation – Step 5.2

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

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





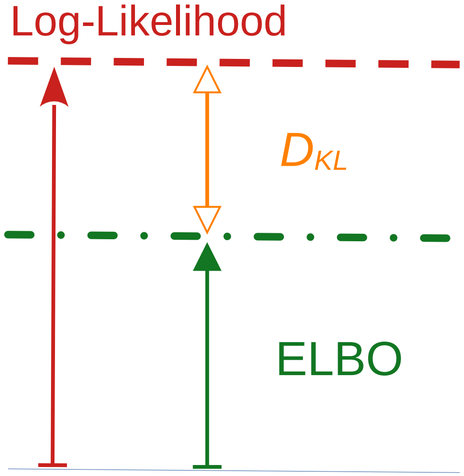
EM Derivation – Step 5.2

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

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

Evidence **L**ower **Bo**und (ELBO)

Evidence ≡ log-likelihood



EM Derivation – Step 5

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

EM Derivation – Step 6

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

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

Intractable!

Direction solution does not work!

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

Intractable

Tractable

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

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

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!

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

EM

Tractable

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

EM Derivation – Step 6

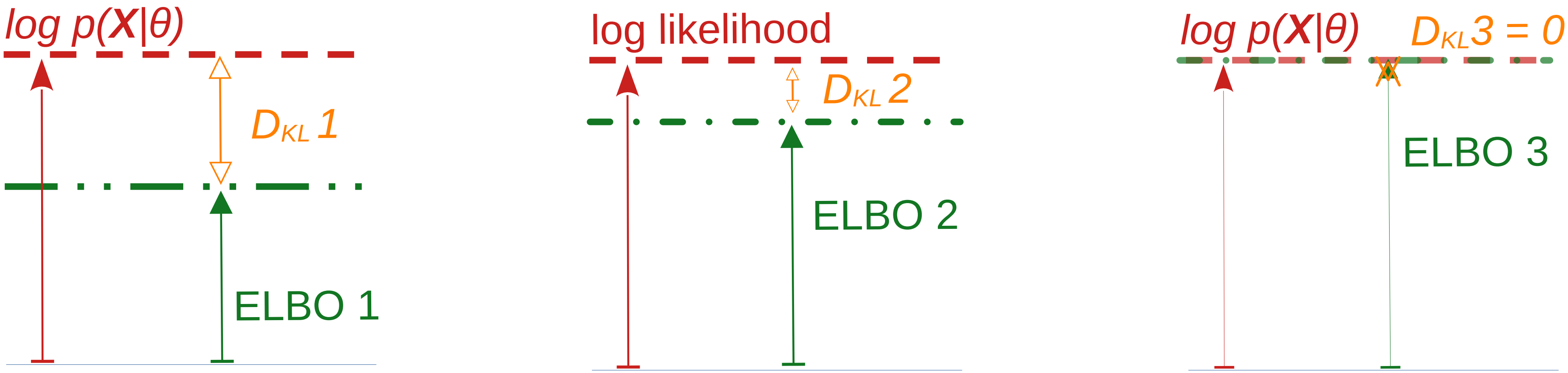
$$\underbrace{\log \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z})}_{\log p(\mathbf{X}|\theta)} = \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{p(\mathbf{X},\mathbf{Z}|\theta)}{q(\mathbf{Z})}\right]}_{ELBO(q,\theta)} + \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{q(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{X},\theta)}\right]}_{D_{KL}(q,\theta)}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

Tractable

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

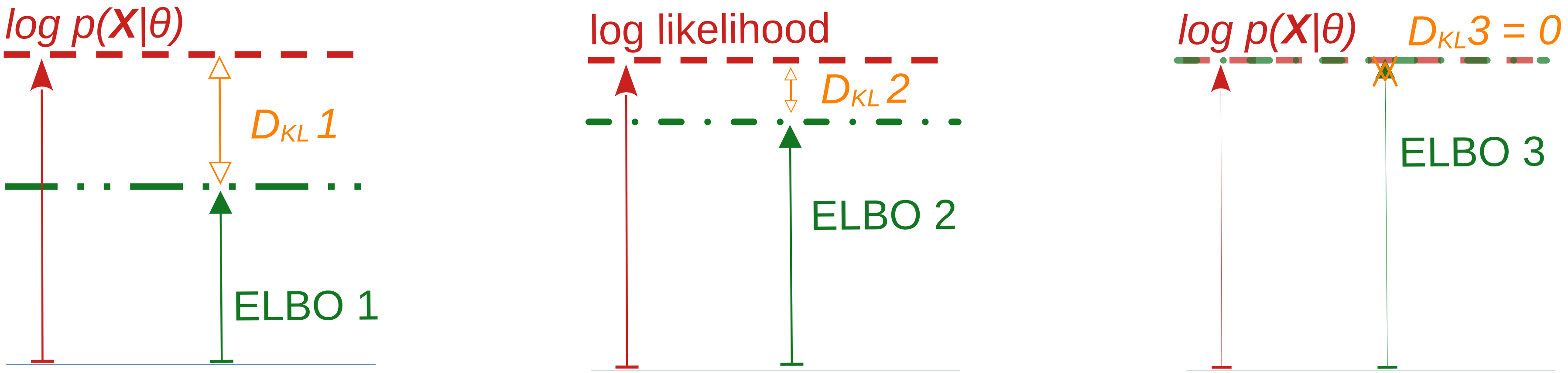
EM → Instead of log-likelihood ... maximise ELBO …

Best ELBO to optimise ...



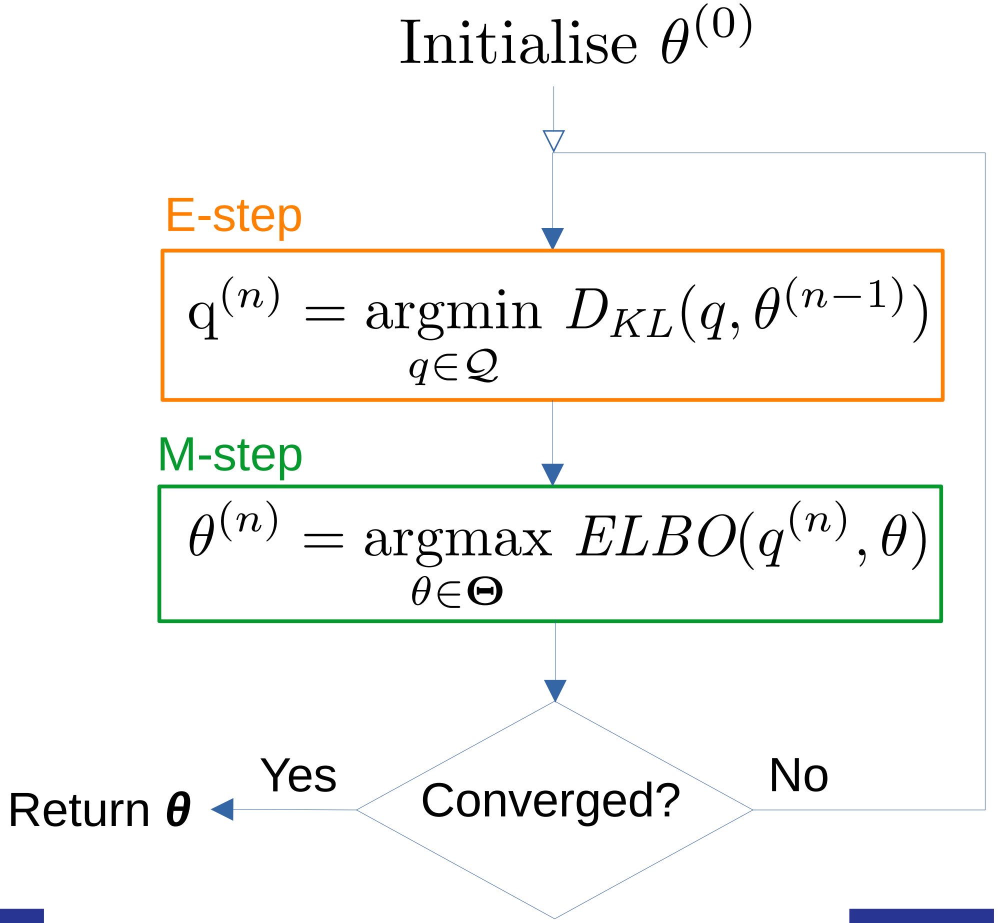
Which ELBO is better?

Best ELBO to optimise ...



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

EM Procedure



Initialise $\theta^{(0)}$

E-step

$$\mathrm{q}^{(n)} = \underset{q\in\mathcal{Q}}{\mathrm{argmin}}\ D_{KL}(q,\theta^{(n-1)})$$

M-step

$$\theta^{(n)} = \underset{\theta\in\boldsymbol{\Theta}}{\mathrm{argmax}}\ ELBO(q^{(n)},\theta)$$

Converged?

Yes

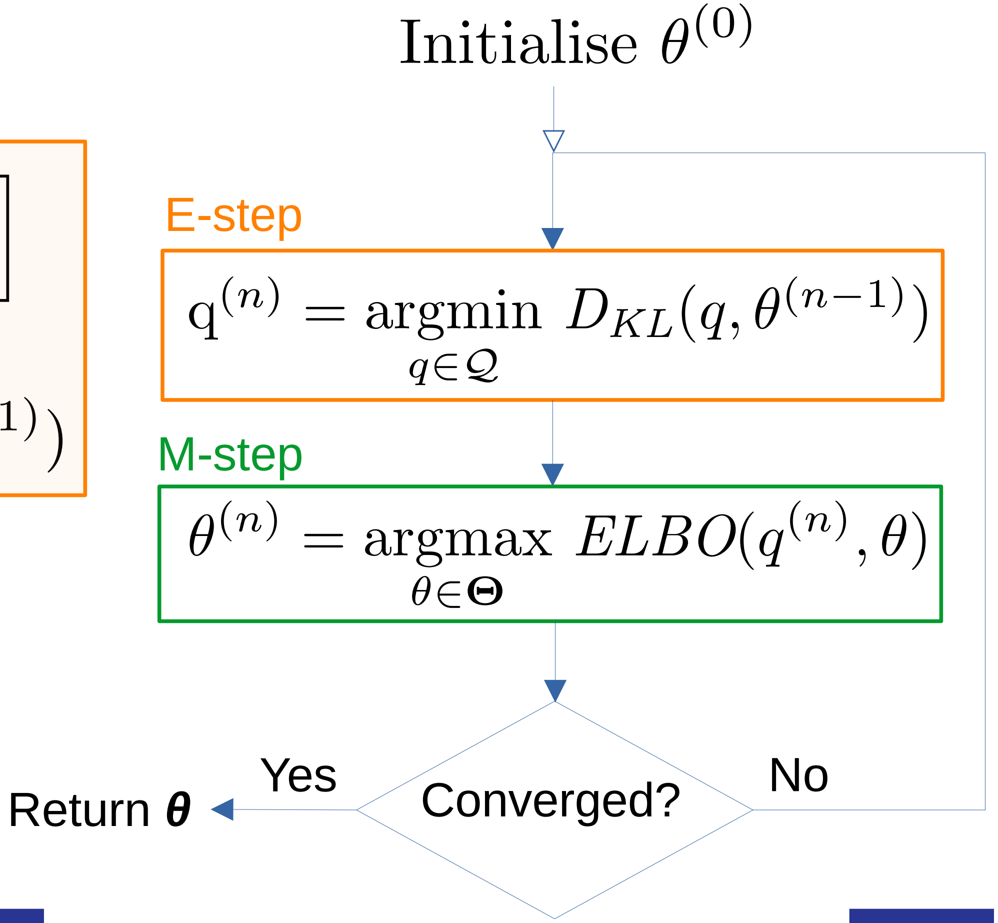
No

Return $\boldsymbol{\theta}$

E-Step

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

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



Initialise $\theta^{(0)}$

E-step

$$\mathrm{q}^{(n)} = \underset{q\in\mathcal{Q}}{\operatorname{argmin}}\ D_{KL}(q,\theta^{(n-1)})$$

M-step

$$\theta^{(n)} = \underset{\theta\in\boldsymbol{\Theta}}{\operatorname{argmax}}\ ELBO(q^{(n)},\theta)$$

Converged?

Yes

Return $\boldsymbol{\theta}$

No

M-Step

$$
\begin{aligned}
ELBO(q^{(n)}, \theta) &= \sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log \left[\frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q^{(n)}(\mathbf{Z})} \right] \\
&= \sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z}|\theta) - \underbrace{\sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log q^{(n)}(\mathbf{Z})}_{\text{constant}}
\end{aligned}
$$

M-Step

$$
\begin{aligned}
ELBO(q^{(n)}, \theta) &= \sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log \left[\frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q^{(n)}(\mathbf{Z})} \right] \\
&= \sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z}|\theta) - \underbrace{\sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log q^{(n)}(\mathbf{Z})}_{\text{constant}}
\end{aligned}
$$

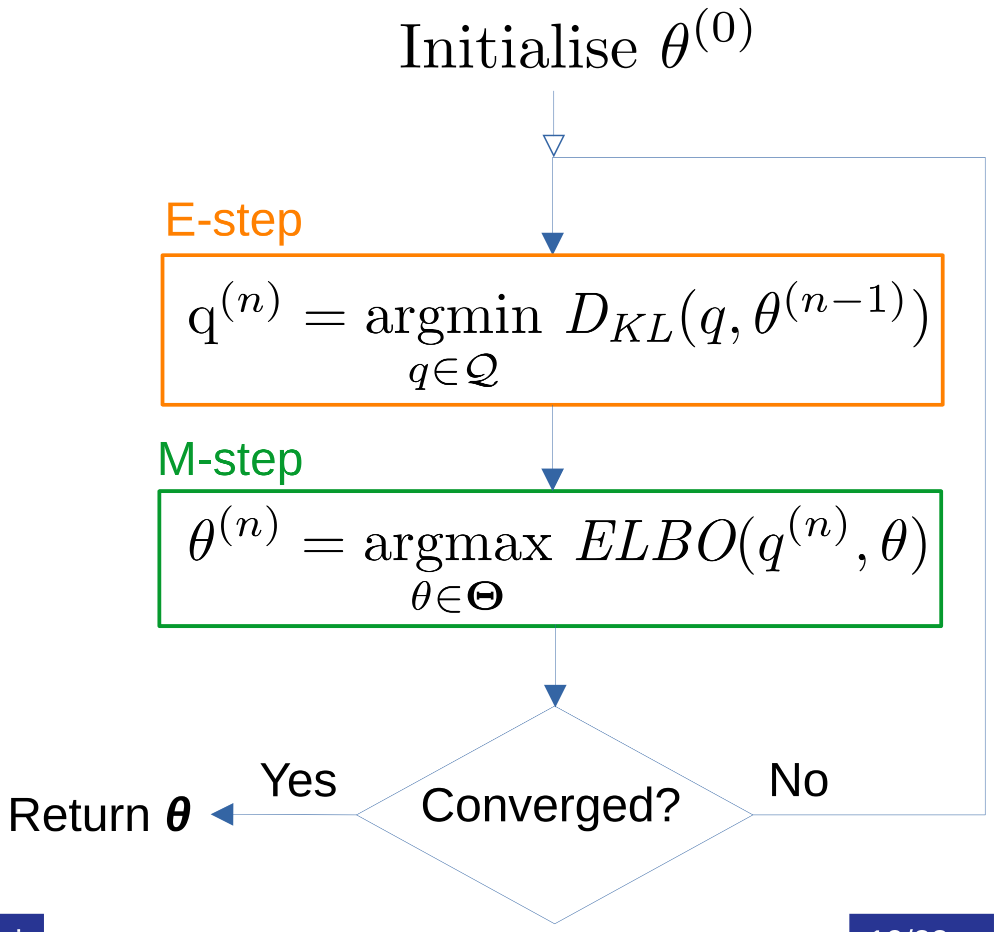
$$
\begin{aligned}
\theta^* &= \operatorname*{argmax}_{\theta \in \Theta} \; ELBO(q^{(n)}, \theta) \\
&= \operatorname*{argmax}_{\theta \in \Theta} \sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z}|\theta)
\end{aligned}
$$

M-Step

M-step

$$\theta^* = \underset{\theta \in \Theta}{\operatorname{argmax}}\ ELBO(q^{(n)}, \theta)$$

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



Initialise $\theta^{(0)}$

E-step

$$\mathrm{q}^{(n)} = \underset{q \in \mathcal{Q}}{\operatorname{argmin}}\ D_{KL}(q, \theta^{(n-1)})$$

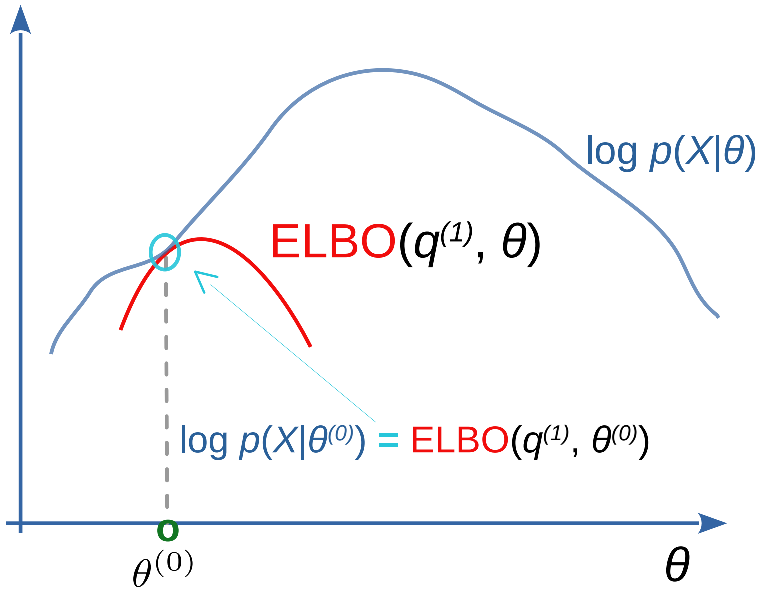
M-step

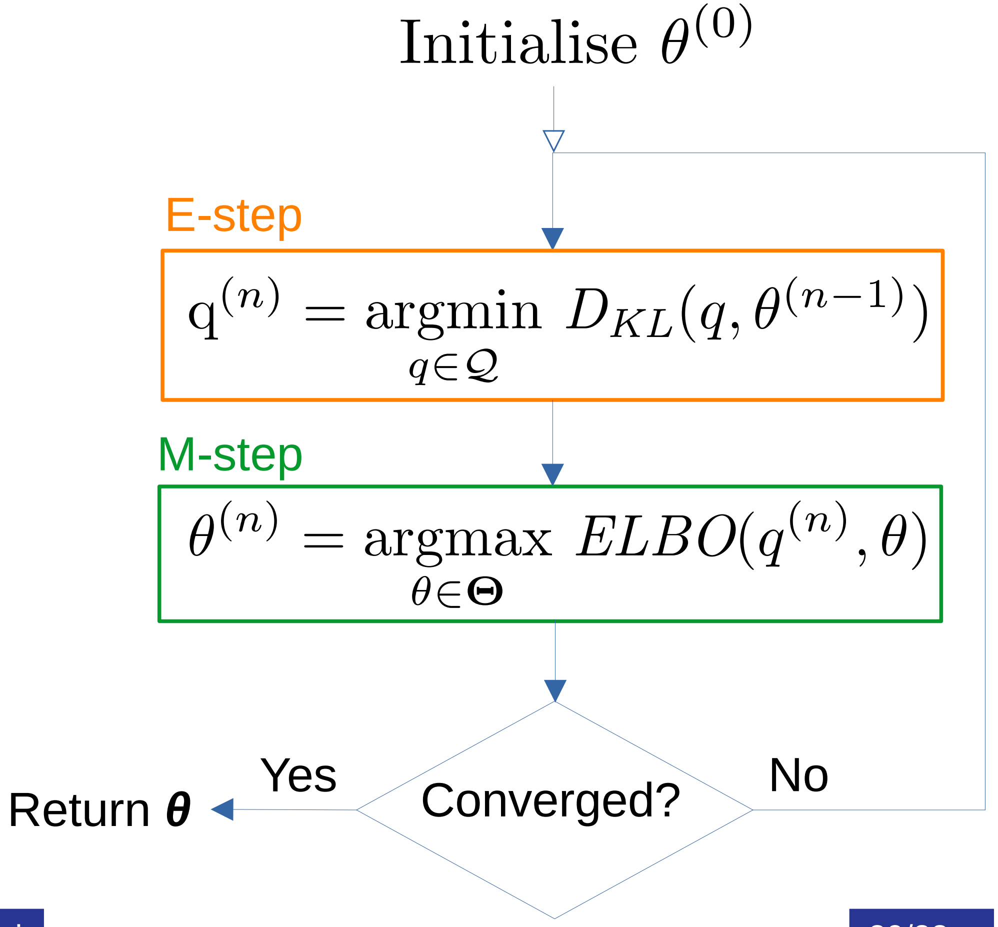
$$\theta^{(n)} = \underset{\theta \in \boldsymbol{\Theta}}{\operatorname{argmax}}\ ELBO(q^{(n)}, \theta)$$

Return $\boldsymbol{\theta}$

Visualisation

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





Initialise $\theta^{(0)}$

E-step

$$\mathrm{q}^{(n)} = \underset{q \in \mathcal{Q}}{\operatorname{argmin}}\ D_{KL}(q, \theta^{(n-1)})$$

M-step

$$\theta^{(n)} = \underset{\theta \in \boldsymbol{\Theta}}{\operatorname{argmax}}\ ELBO(q^{(n)}, \theta)$$

Converged?

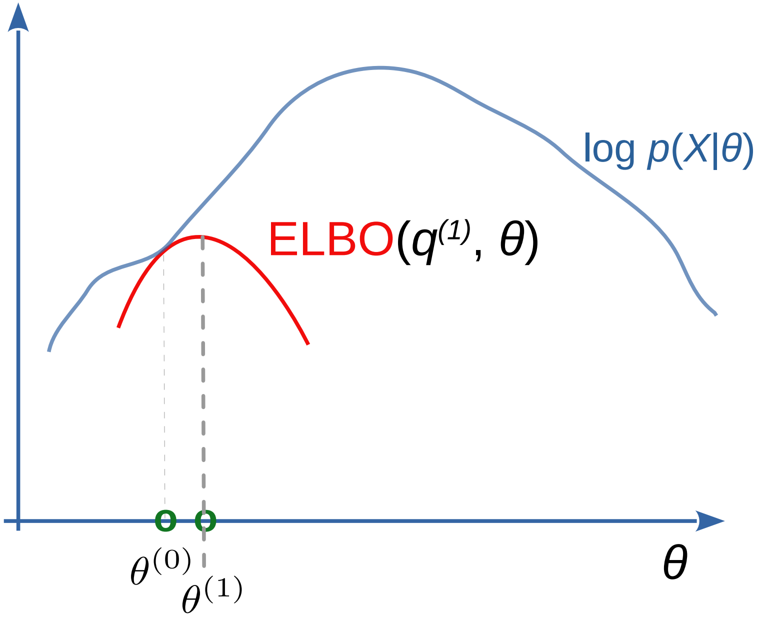
Yes

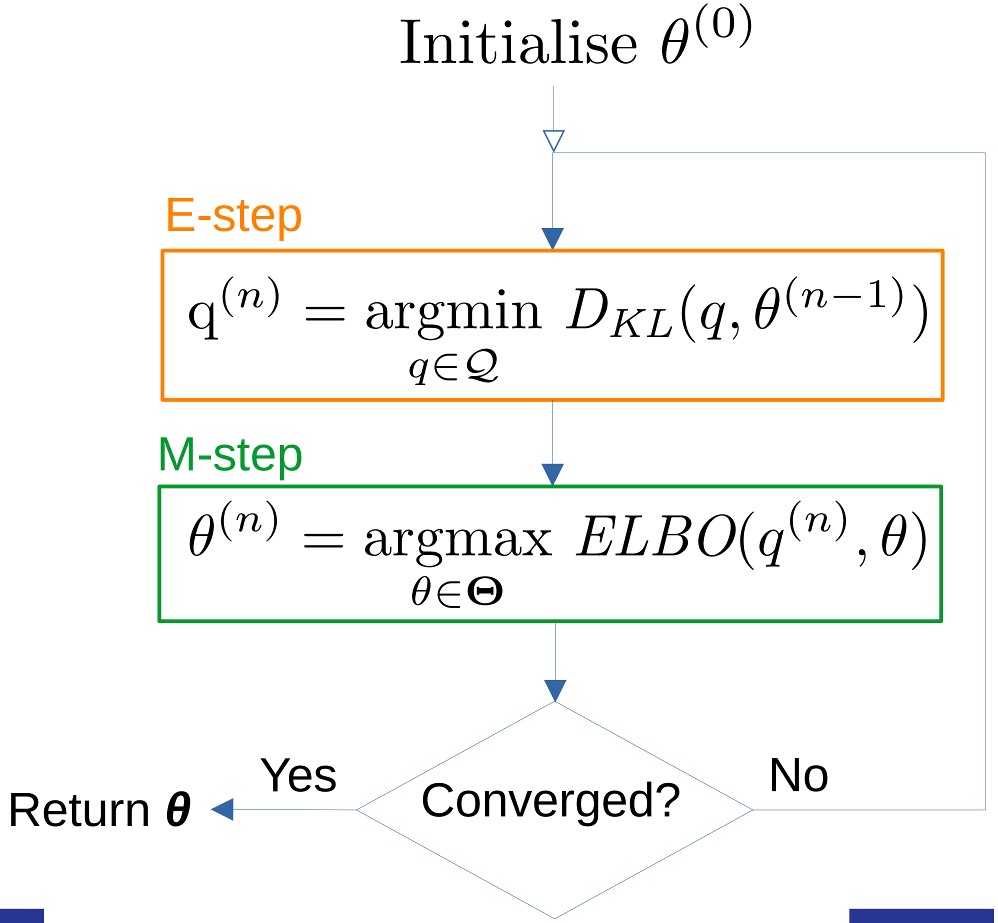
Return $\boldsymbol{\theta}$

No

Visualisation

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





Initialise $\theta^{(0)}$

E-step

$$\mathrm{q}^{(n)} = \underset{q \in \mathcal{Q}}{\operatorname{argmin}} \ D_{KL}(q, \theta^{(n-1)})$$

M-step

$$\theta^{(n)} = \underset{\theta \in \boldsymbol{\Theta}}{\operatorname{argmax}} \ ELBO(q^{(n)}, \theta)$$

Converged?

Yes

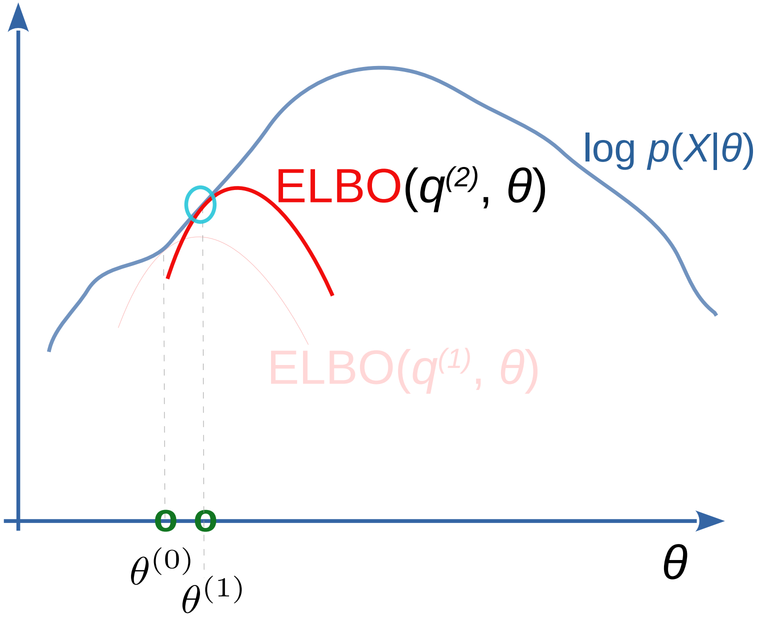
Return $\boldsymbol{\theta}$

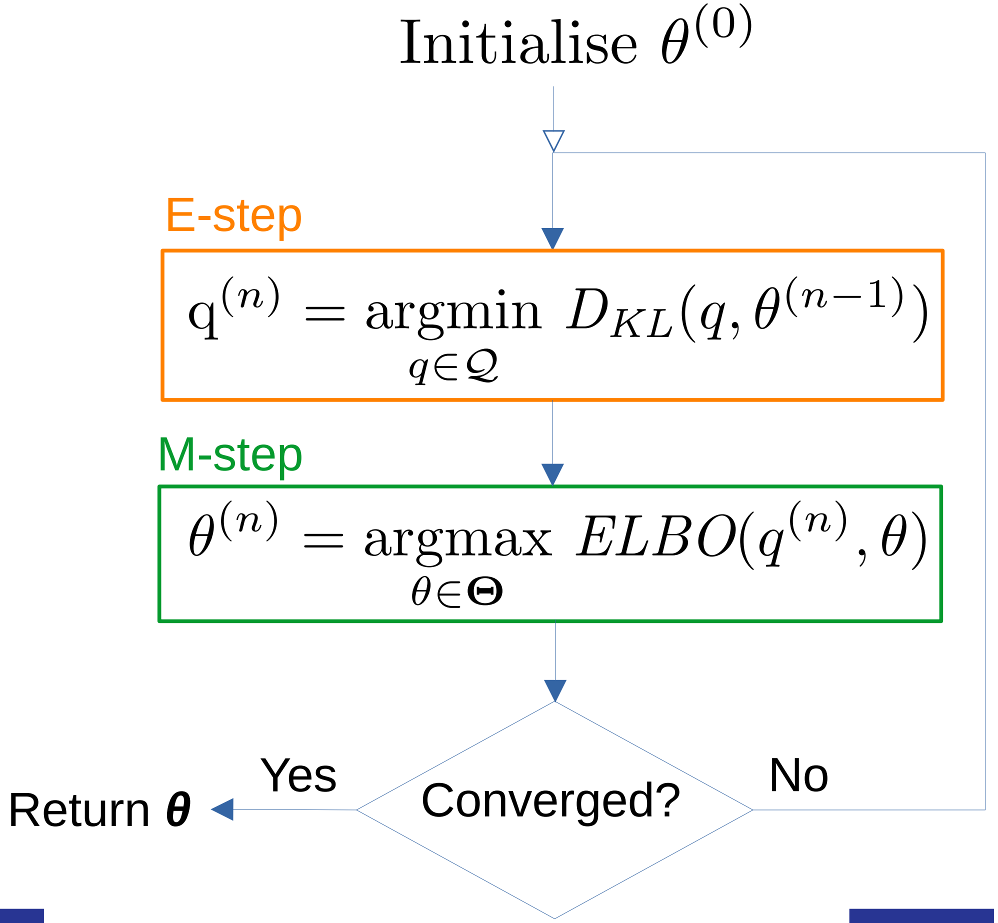
No

Visualisation

E-step: $q^{(2)} = \text{argmin } D_{KL}(q, \theta^{(1)})$

$\log p(X|\theta^{(1)}) = \text{ELBO}(q^{(2)}, \theta^{(1)})$





Initialise $\theta^{(0)}$

E-step

$$\mathrm{q}^{(n)} = \underset{q \in \mathcal{Q}}{\text{argmin}} \; D_{KL}(q, \theta^{(n-1)})$$

M-step

$$\theta^{(n)} = \underset{\theta \in \boldsymbol{\Theta}}{\text{argmax}} \; ELBO(q^{(n)}, \theta)$$

Converged?

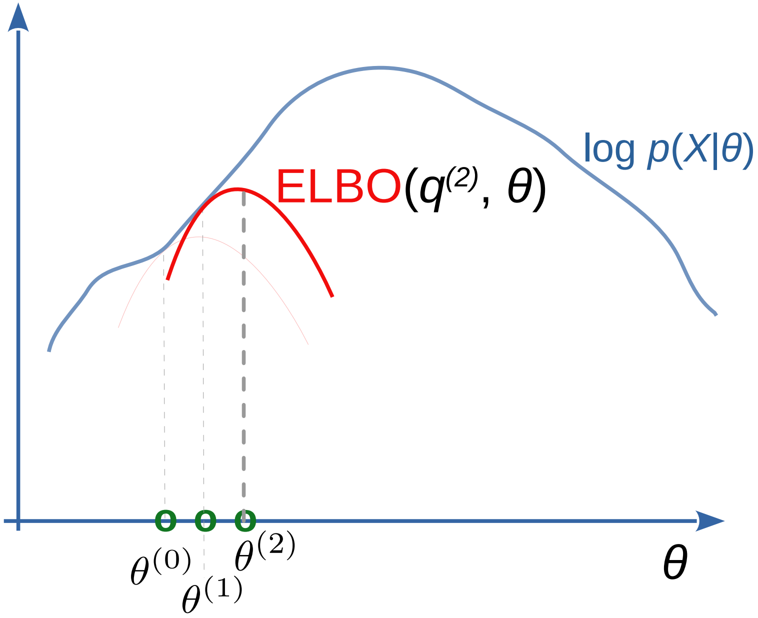
Yes

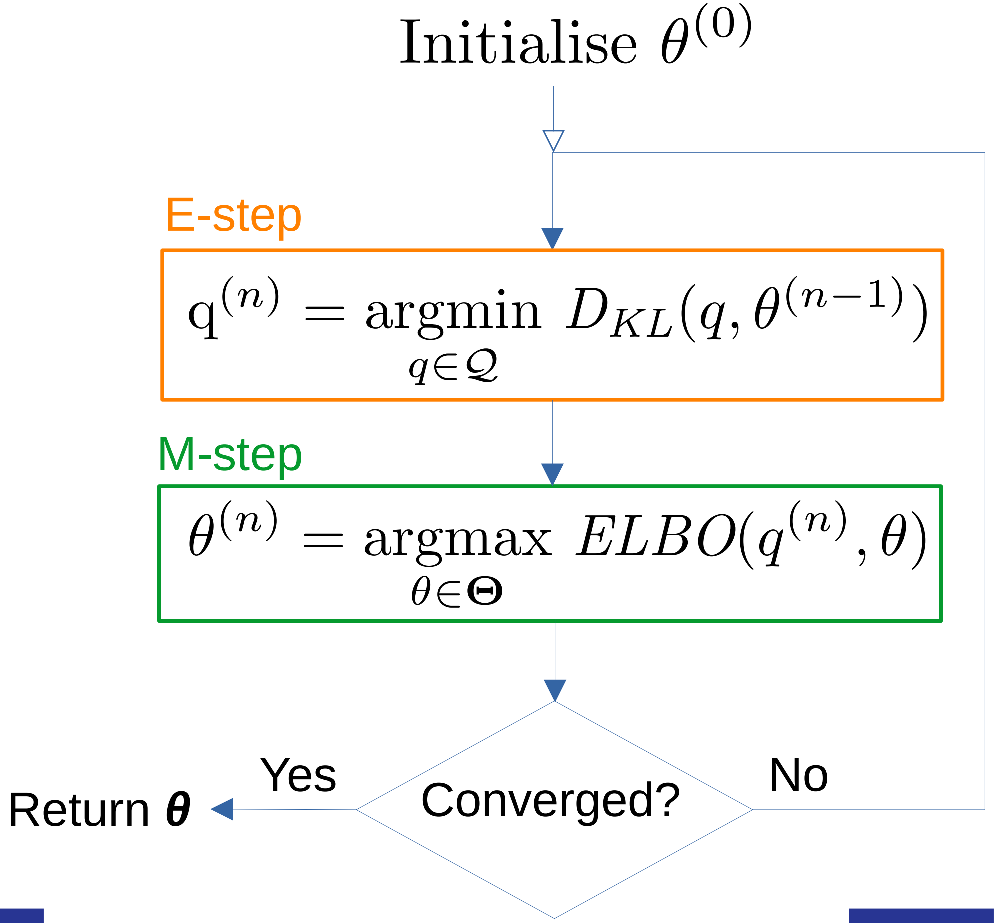
No

Return $\boldsymbol{\theta}$

Visualisation

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





Initialise $\theta^{(0)}$

E-step

$$q^{(n)} = \underset{q \in \mathcal{Q}}{\text{argmin}}\ D_{KL}(q, \theta^{(n-1)})$$

M-step

$$\theta^{(n)} = \underset{\theta \in \boldsymbol{\Theta}}{\text{argmax}}\ ELBO(q^{(n)}, \theta)$$

Converged?

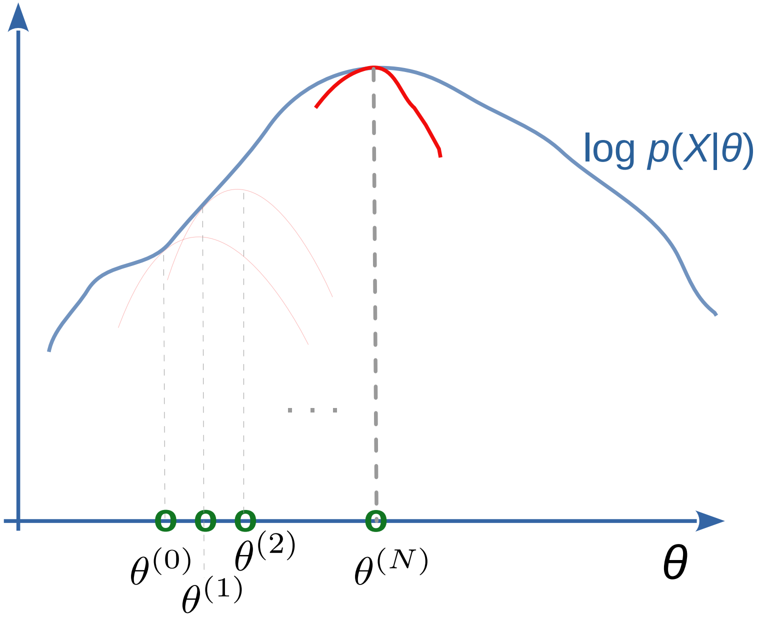
Yes

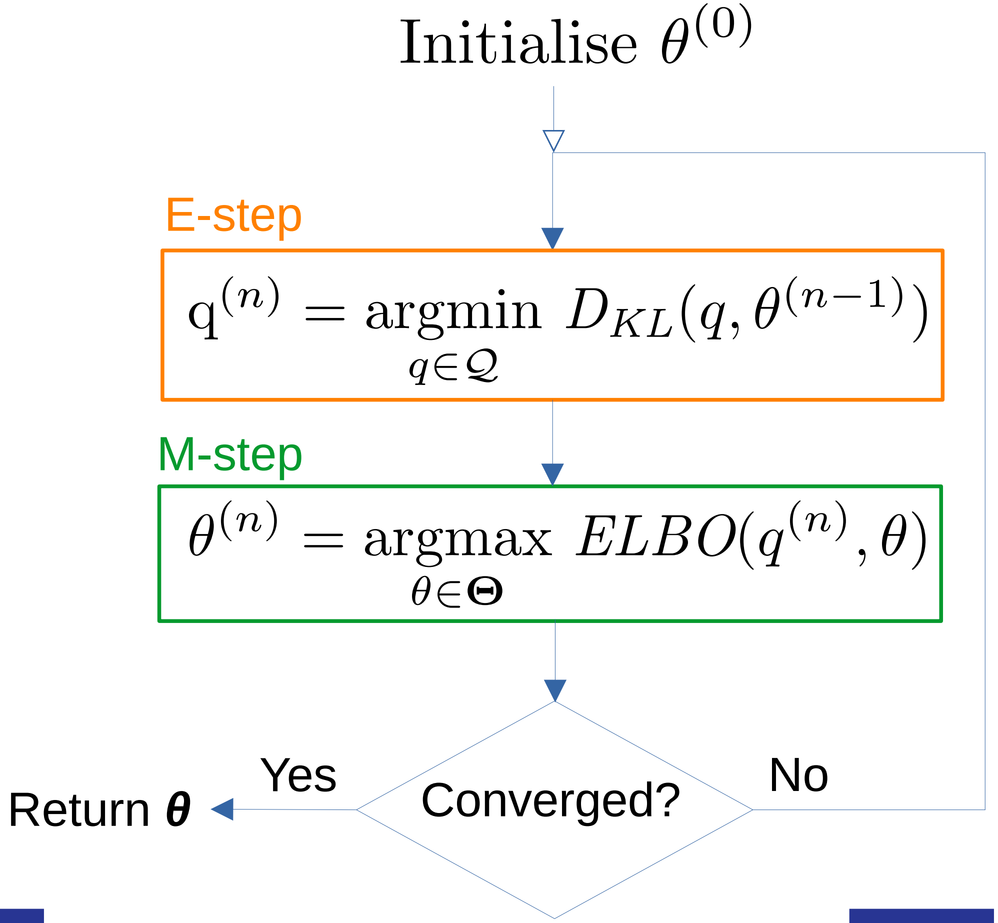
No

Return $\boldsymbol{\theta}$

Visualisation

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





Initialise $\theta^{(0)}$

E-step

$$\mathrm{q}^{(n)} = \underset{q \in \mathcal{Q}}{\operatorname{argmin}} \; D_{KL}(q, \theta^{(n-1)})$$

M-step

$$\theta^{(n)} = \underset{\theta \in \boldsymbol{\Theta}}{\operatorname{argmax}} \; ELBO(q^{(n)}, \theta)$$

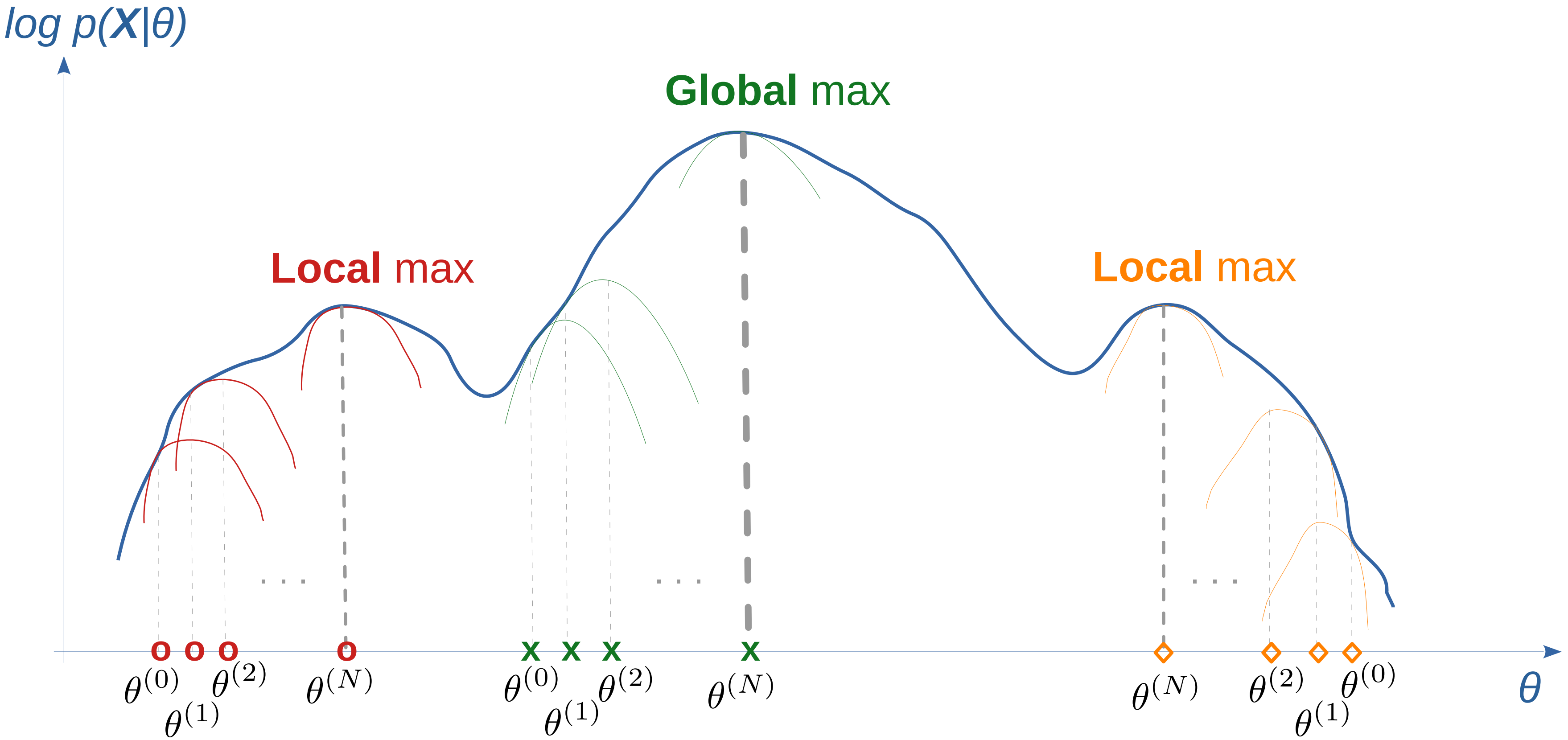
Converged?

Yes

Return $\boldsymbol{\theta}$

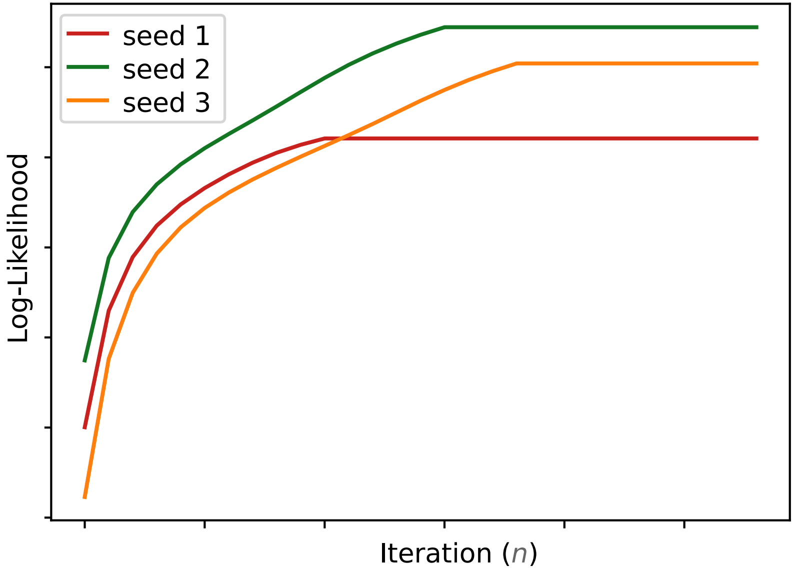
No

Initialisation Matters …



Initialisation Matters ...

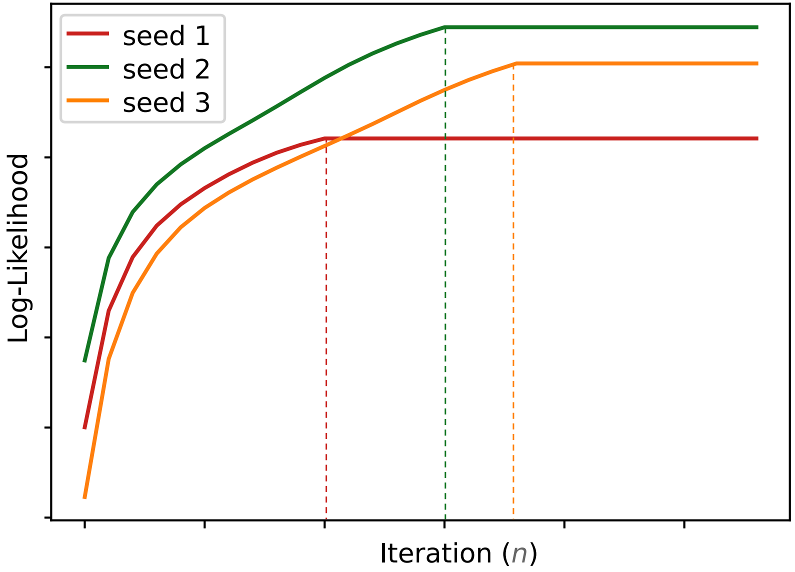
- $p(\mathbf{X}|\theta^{(n)})$ is **ALWAYS** non-decreasing



Initialisation Matters …

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

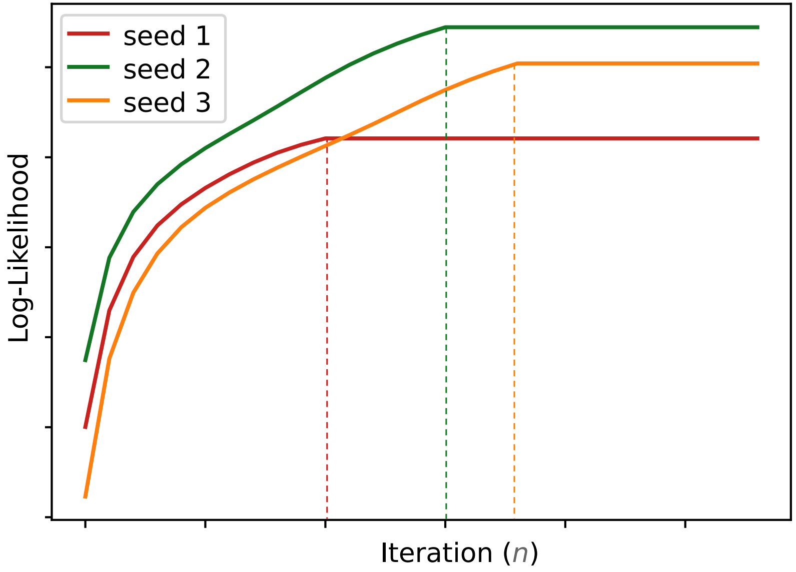
- Initialisation affects … convergence rate and final log-likelihood



Initialisation Matters ...

- $p(\mathbf{X}|\theta^{(n)})$ is **ALWAYS** non-decreasing
- Initialisation affects ... convergence rate and **final log-likelihood**

Try multiple initialisations, pick up the **best** model.



Wrap-up … EM ...

- **Goal**: estimate $\boldsymbol{\theta}_{ML}$ for probabilistic models with latent var
- **How**: an iterative two-stage (E-step, M-step) procedure
- **Assignment**: estimate $\boldsymbol{\theta}_{MAP}$ using EM
- **Applications**: GMM, HMM, Computational biology, etc.

- **Next session**: ...

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