Expectation Maximisation (EM)

Erfan Loweimi

https://eloweimi.github.io

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

This seminal paper was **NOT** the first to discover EM but rather ...

- Generalised it beyond special circumstances/applications
- Sketched a convergence analysis

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

independent

identically distributed

$$p(\mathbf{X}|\theta) = p(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N|\theta) \overset{i.i.d}{=} \prod_{i=1}^{N} p(\mathbf{x}_i|\theta)$$

$$\log p(\mathbf{X}|\theta) = \sum_{i=1}^{N} \log p(\mathbf{x}_i|\theta)$$

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

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

Setup

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

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

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

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 ...

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

Find $\boldsymbol{\theta}_{ML}$ such that the likelihood of data **X**, being generated by Model $\boldsymbol{\theta}$, is maximised.

Goal ...

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

- We prefer maximising **log**-likelihood ...
  - **Note**: log is *strictly increasing* → argmax f(x) = argmax log(f(x))
  - **Advantages**:
    - ✓ Mathematical convenience → log(exp[.]) = [.]
    - ✓ Numerical stability

Goal ...

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

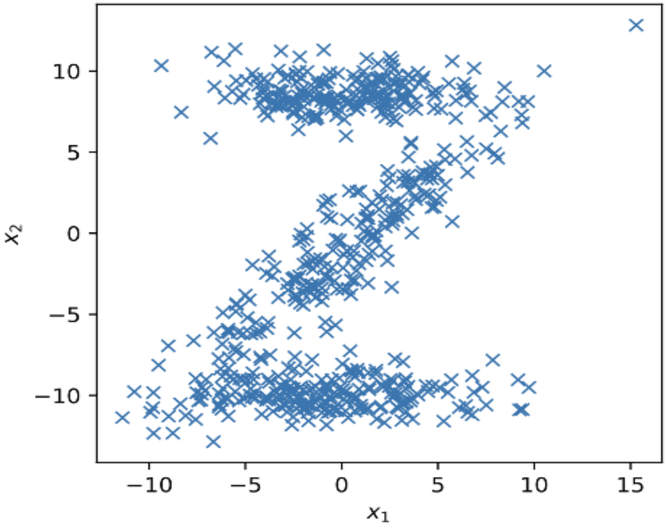
$$= \underset{\theta \in \Theta}{\operatorname{argmax}} \; \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\theta)$$

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

Latent Variable (Z)

Incomplete data (X)

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

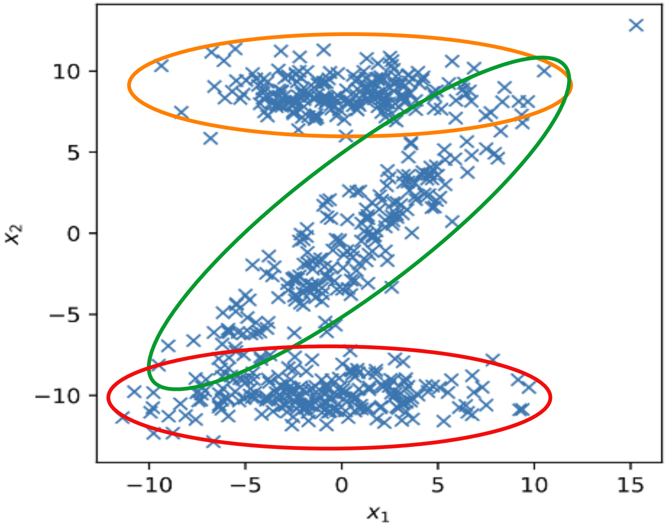


Interpretation: *latent variable* is a part of a model ... *explains* ***X***.

Latent Variable (Z)

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

Incomplete data (X)



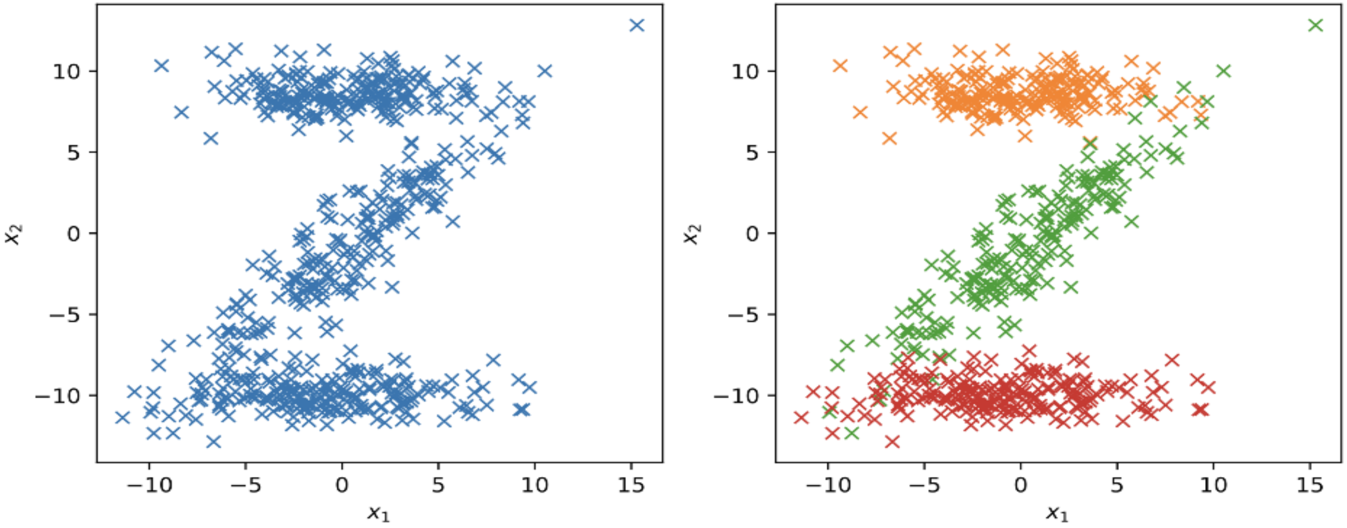
Consider clustering ...

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

Direct Solution

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

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

Step 1 Step 2

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

Step 3

θ_0: derivative roots

Direct Solution

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

Intractable (no closed-form solution!)

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

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

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 a simple case ... Gaussian

Intractable

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

How about *numerical methods*? Slow and do not scale!

Direction solution does not work!

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

… = 0 → Intractable

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

$$\neq$$

Optimise … θ*

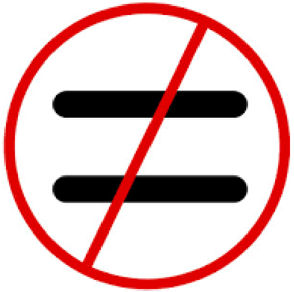
$$\sum_{\mathbf{Z}} \log p(\mathbf{X}, \mathbf{Z}|\theta)$$

Tractable

(when *p* belongs to the exponential family)

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*

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

Intractable

Optimise … θ*

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

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

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

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

Step 2: Take *log* from both sides

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

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

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

- *D_{KL} (KL Divergence)* properties:
  - ✓ $D_{KL}(q \,||\, p) \geq 0$
  - ✓ $D_{KL}(q \,||\, p) = 0 \overset{\text{iff}}{\leftrightarrow} q = p$

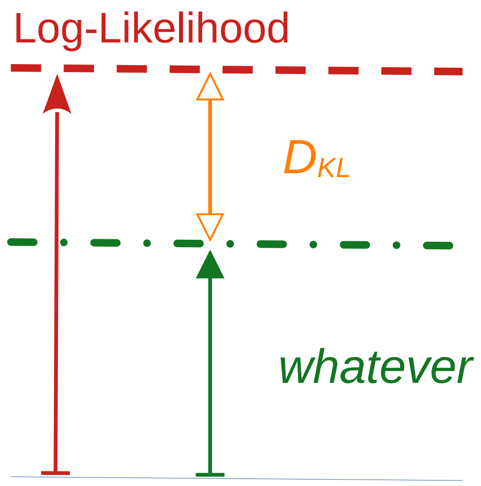
EM Derivation – Step 5.2

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

???

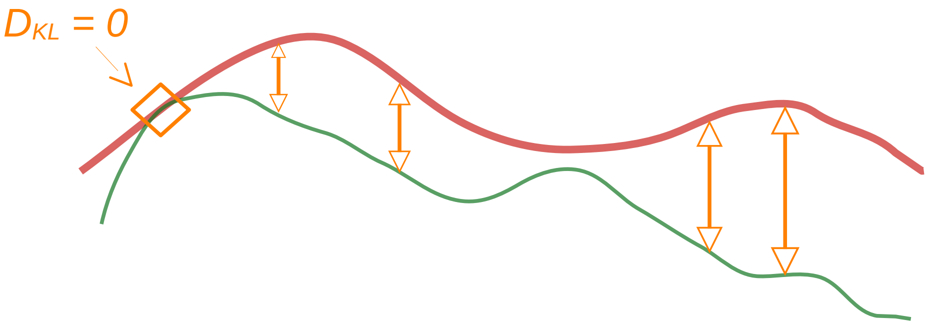
EM Derivation – Step 5.2

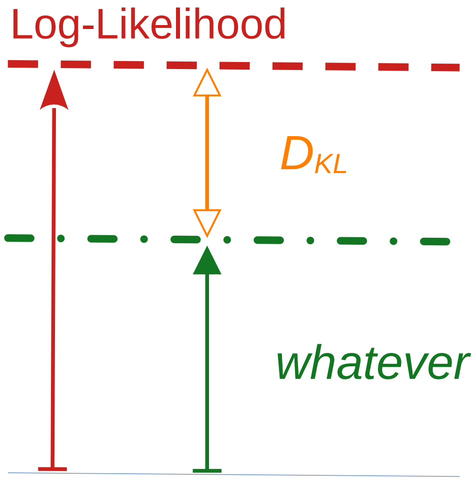
$$\log p(\mathbf{X}|\theta) = \text{whatever} + \underbrace{D_{KL}(q(\mathbf{Z}) \;||\; p(\mathbf{Z}|\mathbf{X},\theta))}_{\geq 0}$$



EM Derivation – Step 5.2

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

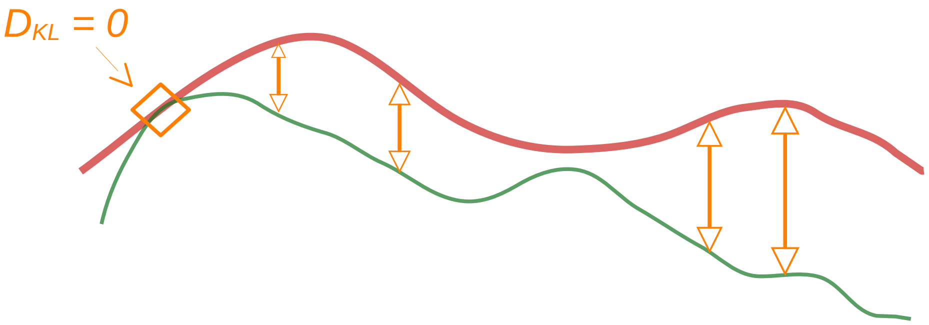


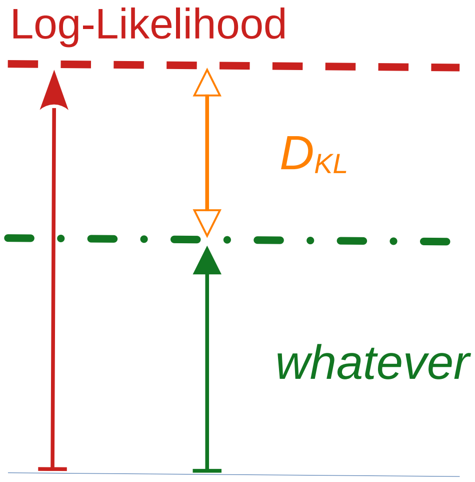


EM Derivation – Step 5.2

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

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





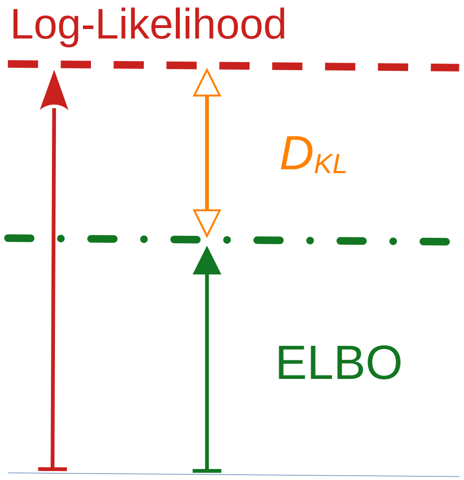
EM Derivation – Step 5.2

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

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

Evidence **L**ower **B**ound (**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

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

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

Intractable!

Direction solution does not work!

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

… = 0 → Intractable

RECALL Slide 9

IFFF we could swap log & Σ …

… = 0 → Tractable

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

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

EM Derivation – Step 5

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

RECALL

EM

Intractable!

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

Tractable

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

EM Derivation – Step 6

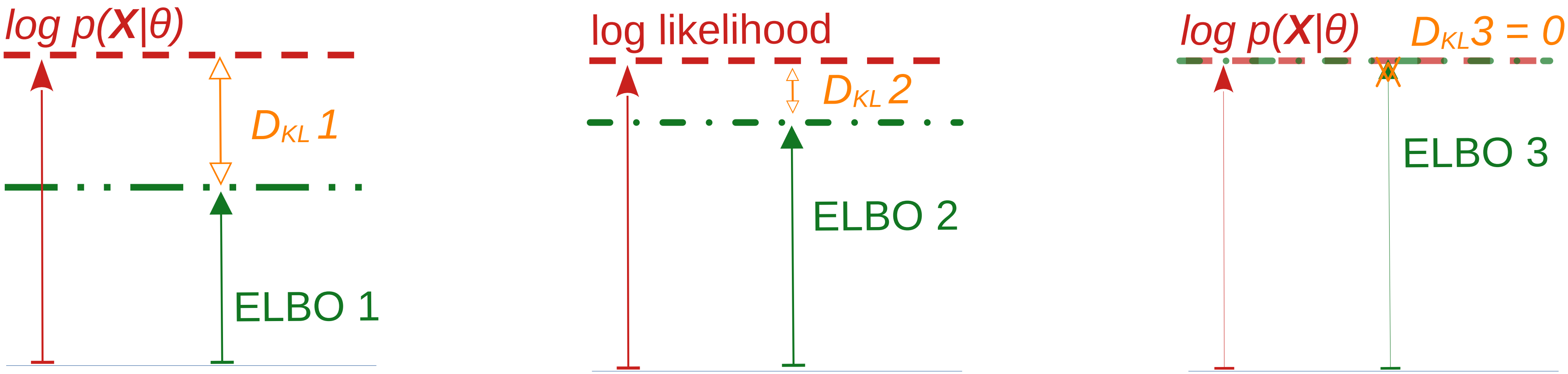
$$\underbrace{\log \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z})}_{\log p(\mathbf{X}|\theta)} = \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{p(\mathbf{X},\mathbf{Z}|\theta)}{q(\mathbf{Z})}\right]}_{ELBO(q,\theta)} + \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{q(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{X},\theta)}\right]}_{D_{KL}(q,\theta)}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

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

Tractable

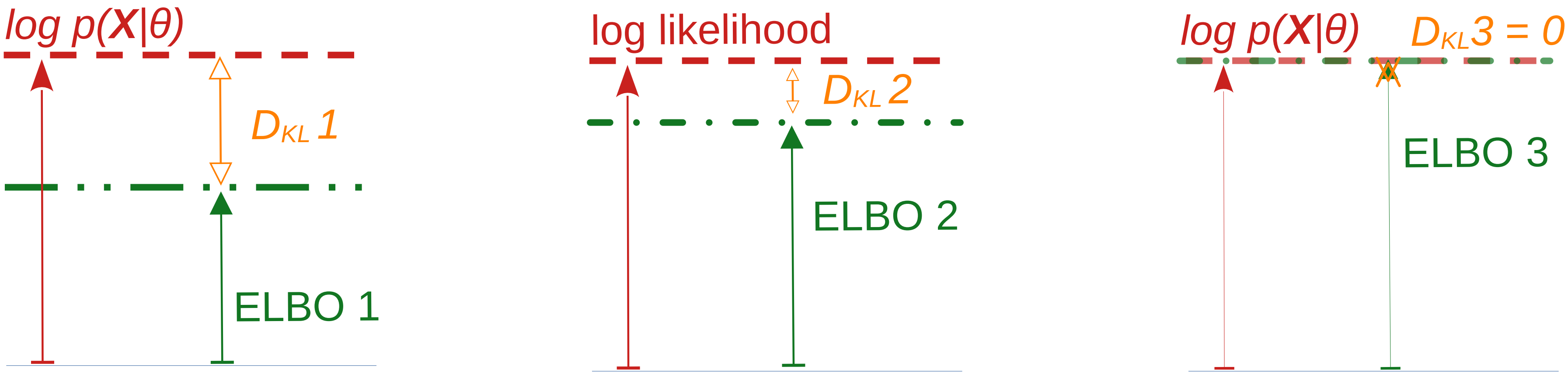
EM → Instead of log-likelihood ... maximise ELBO ...

Best ELBO to optimise ...



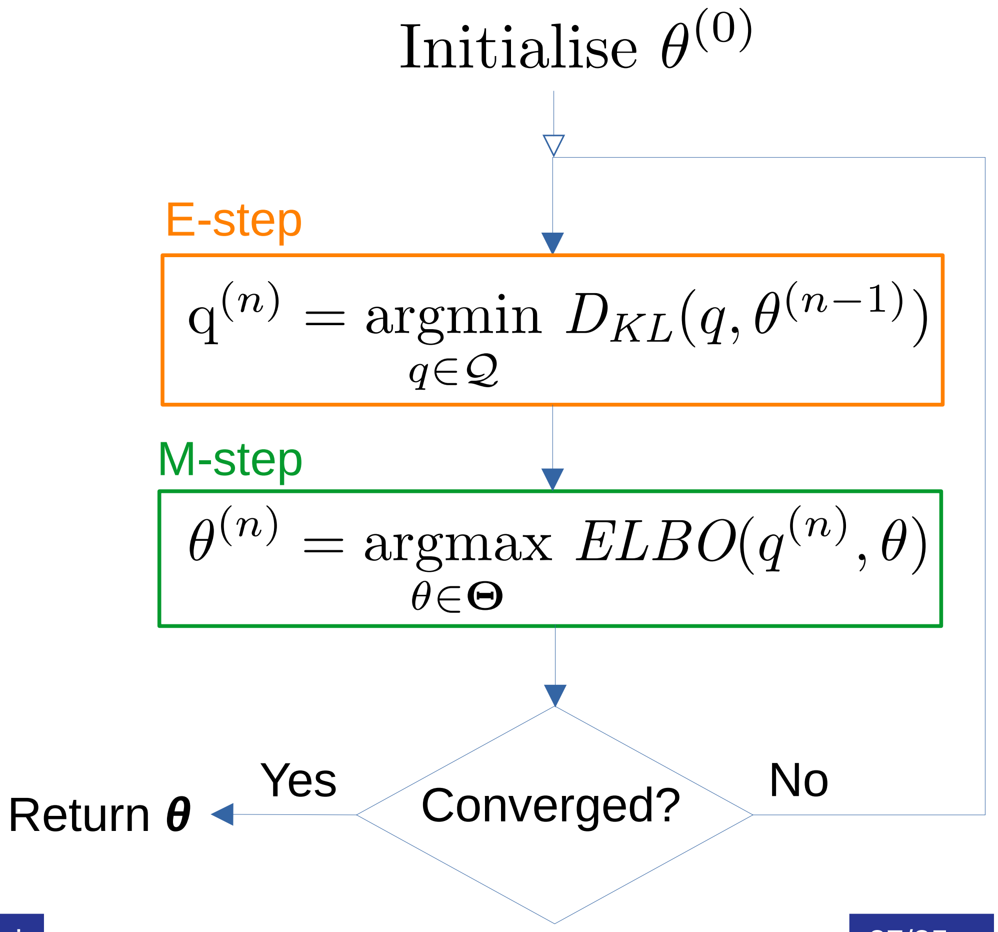
Which ELBO is better?

Best ELBO to optimise ...



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

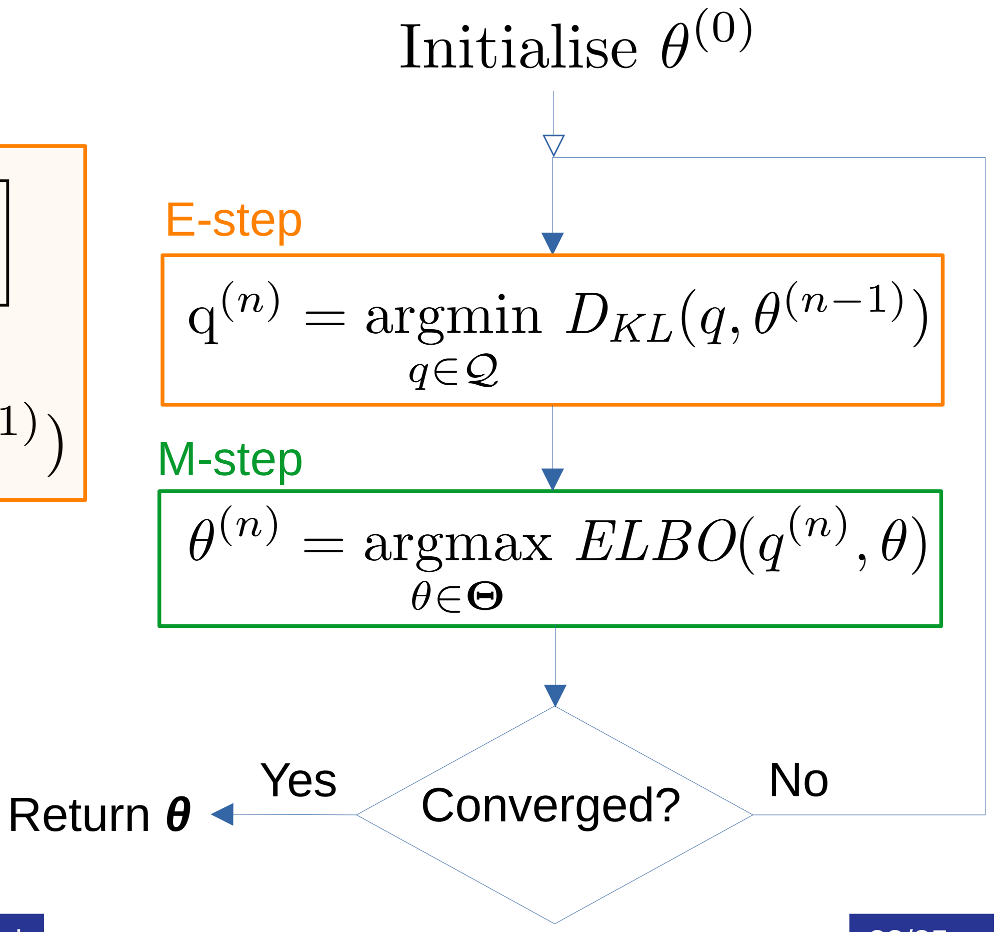
EM Procedure



E-Step

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

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



M-Step

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

$$= \sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z}|\theta) - \underbrace{\sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log q^{(n)}(\mathbf{Z})}_{\text{constant}}$$

M-Step

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

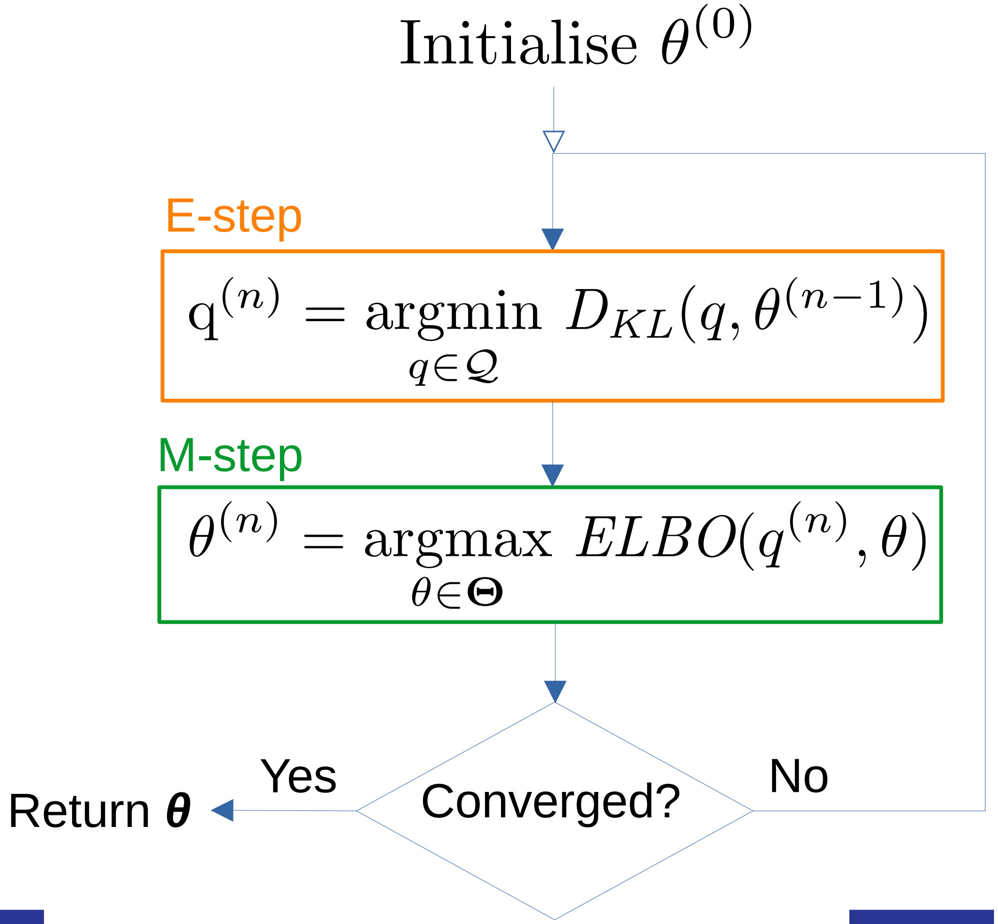
$$
\begin{aligned}
\theta^* &= \underset{\theta \in \Theta}{\operatorname{argmax}}\ ELBO(q^{(n)}, \theta) \\
&= \underset{\theta \in \Theta}{\operatorname{argmax}} \sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z}|\theta)
\end{aligned}
$$

M-Step

M-step

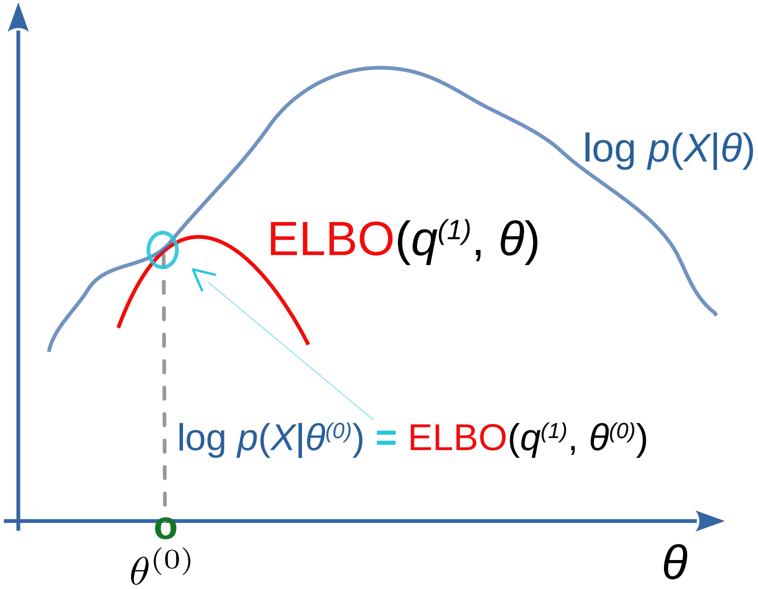
$$\theta^* = \underset{\theta \in \Theta}{\text{argmax}} \; ELBO(q^{(n)}, \theta)$$

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



Visualisation

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



Initialise $\theta^{(0)}$

E-step

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

M-step

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

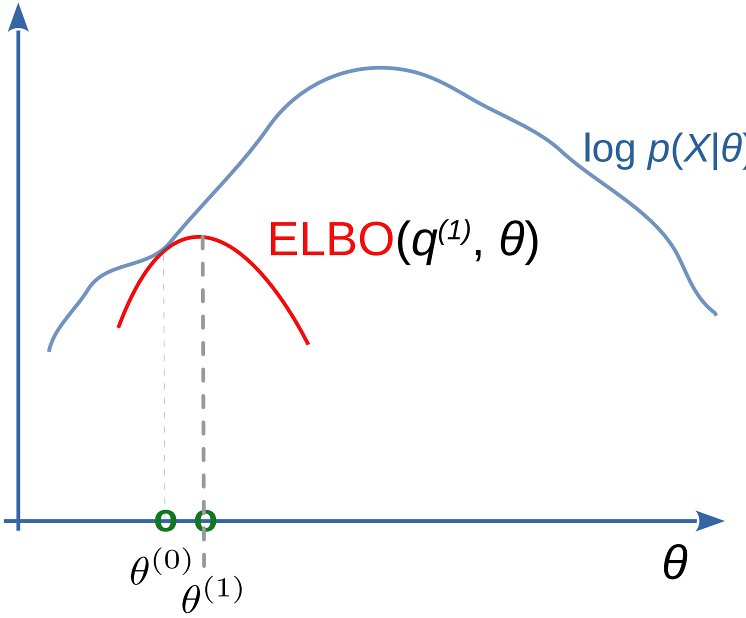
Converged?

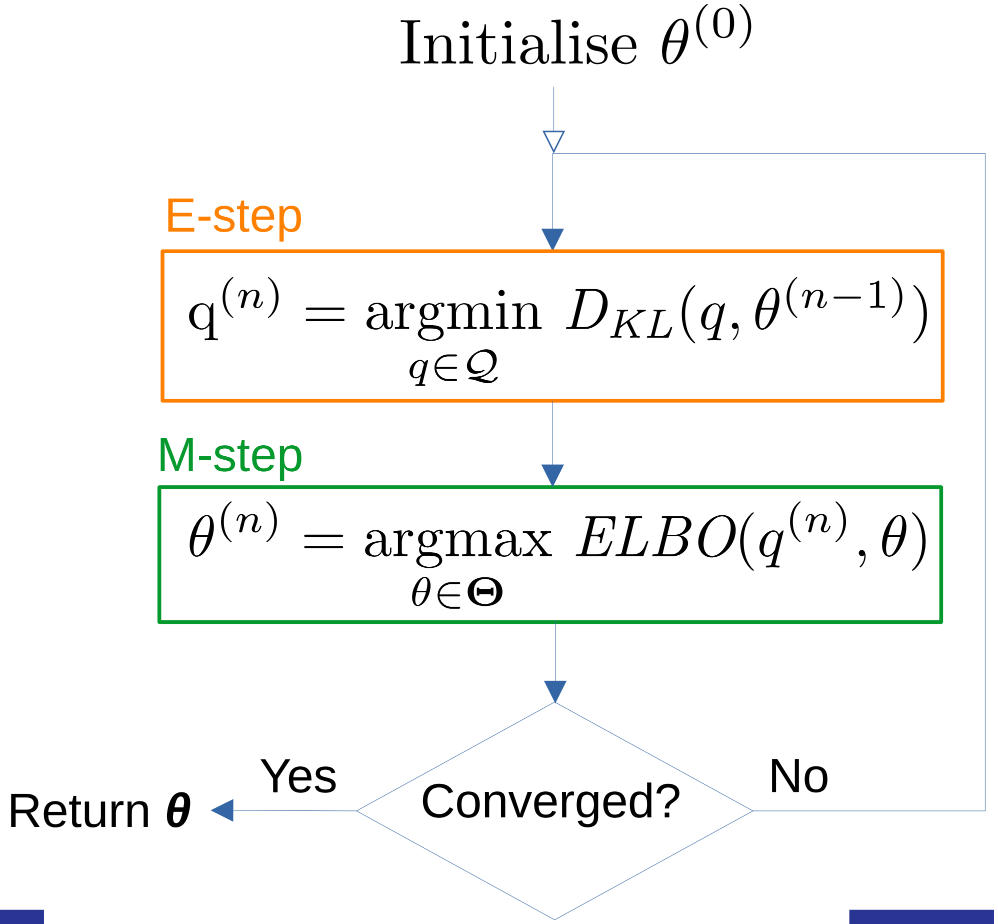
Yes: Return $\boldsymbol{\theta}$

No

Visualisation

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

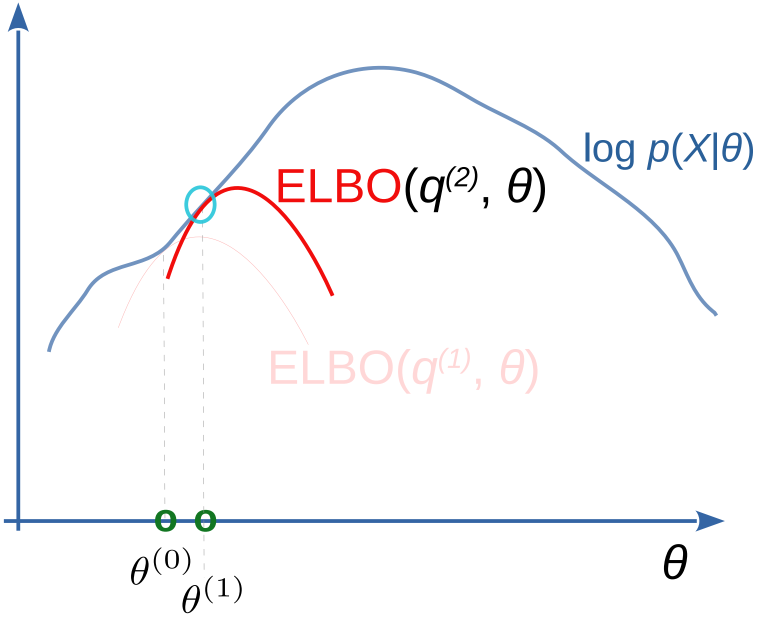


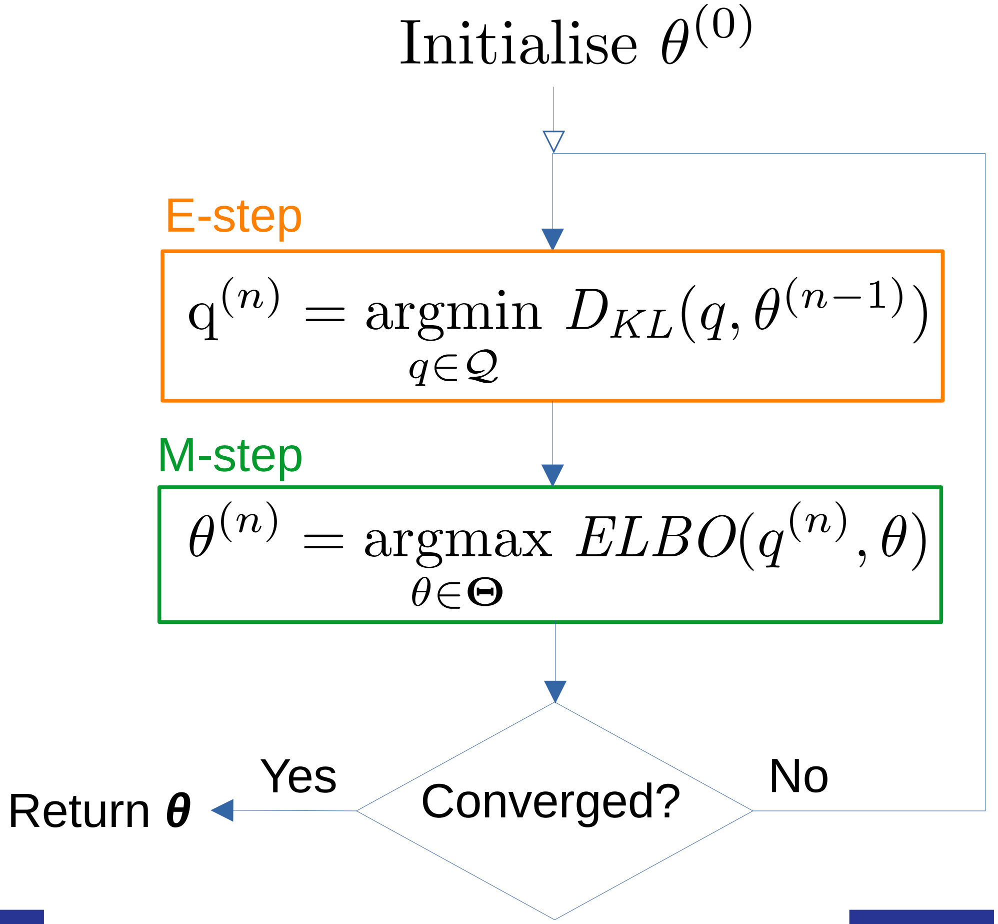


Visualisation

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

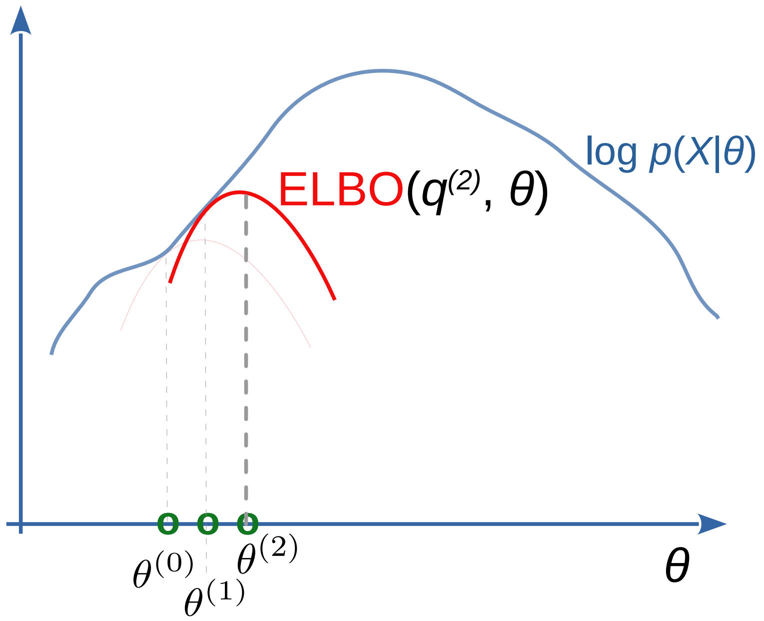
$\log p(X|\theta^{(1)}) = \text{ELBO}(q^{(2)}, \theta^{(1)})$

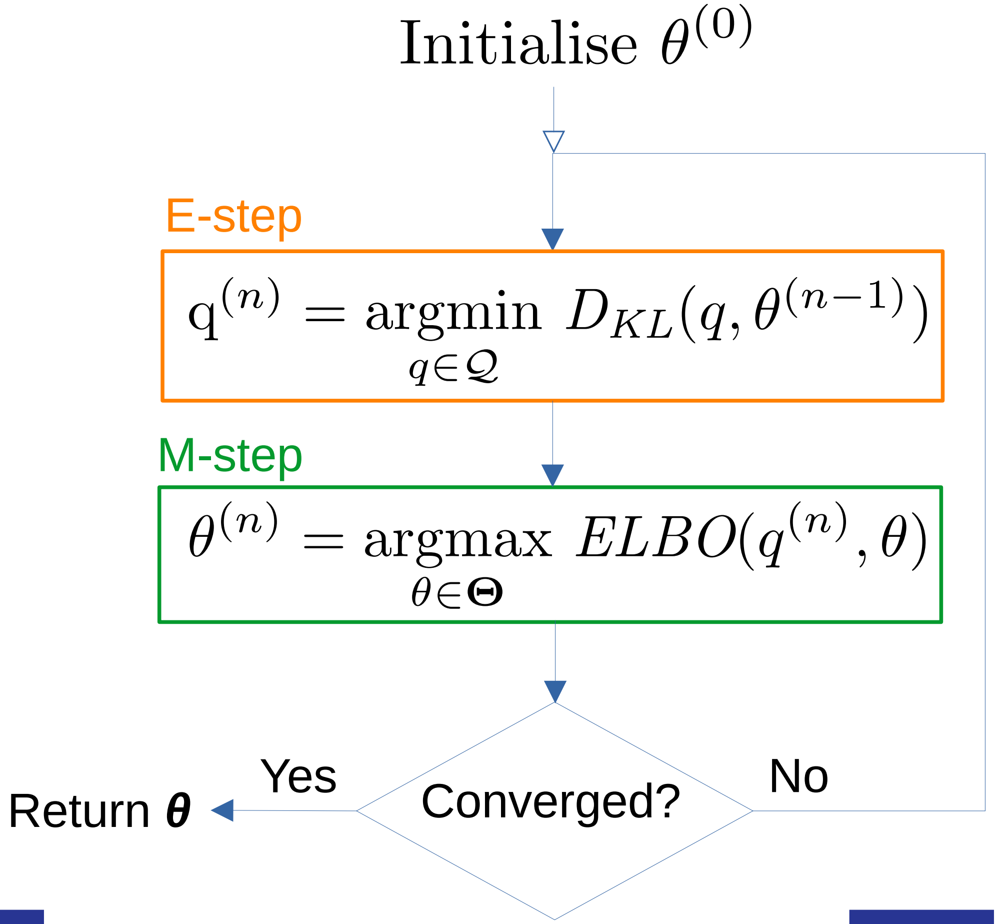




Visualisation

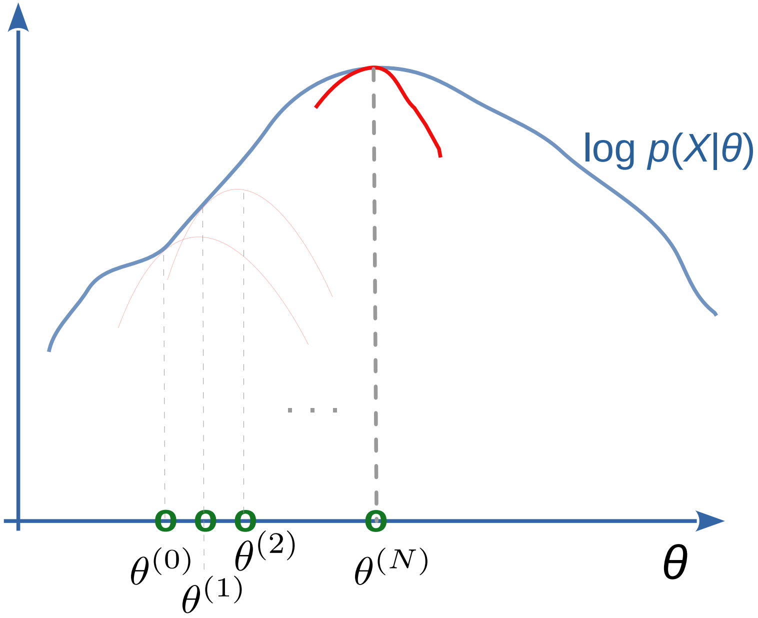
M-step: $\theta^{(2)}$ = argmax ELBO($q^{(2)}$, θ)





Visualisation

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



Initialise $\theta^{(0)}$

E-step

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

M-step

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

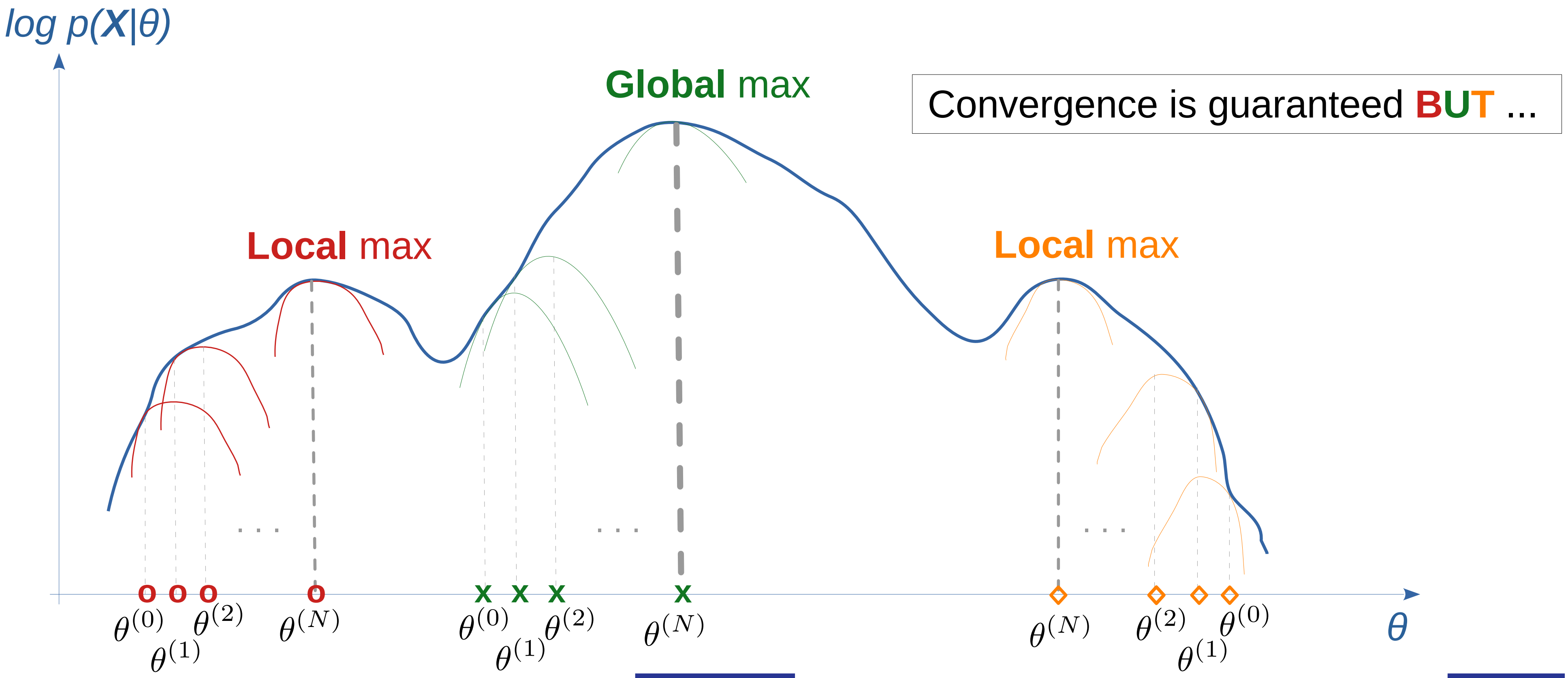
Converged?

Yes

Return $\boldsymbol{\theta}$

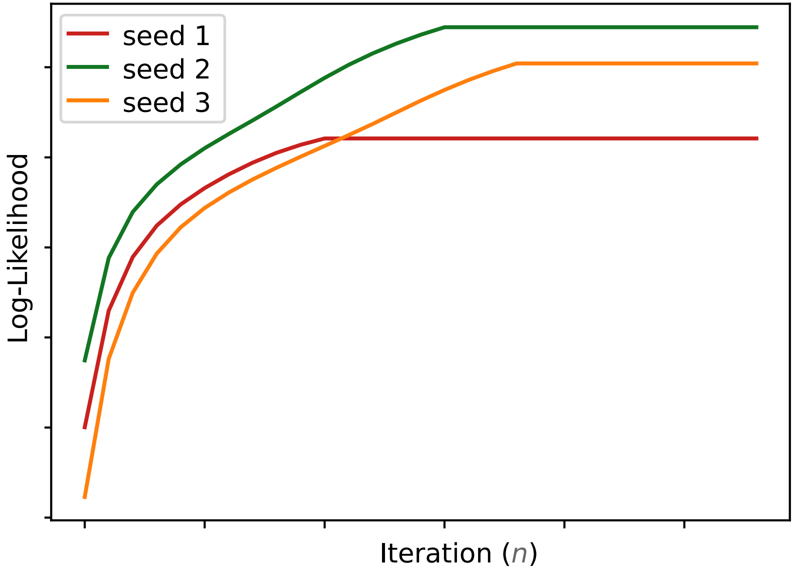
No

Initialisation Matters (1)



Initialisation Matters (2)

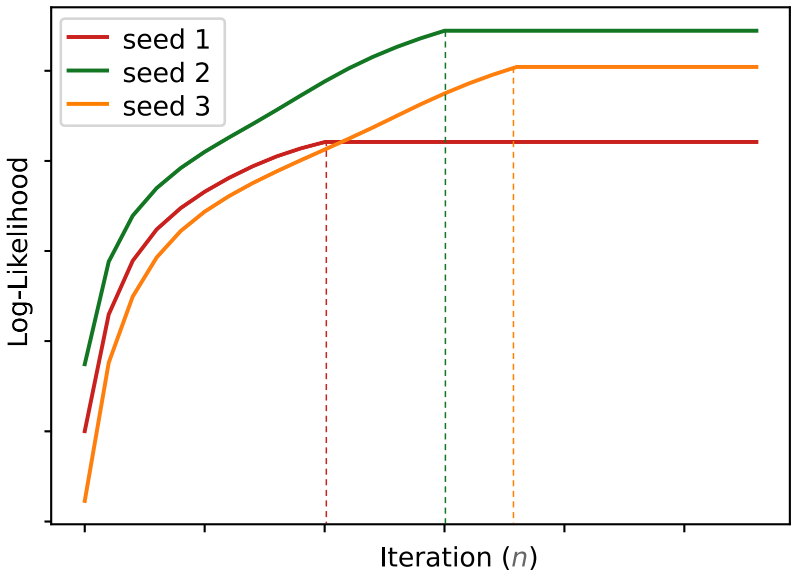
- $p(\mathbf{X}|\theta^{(n)})$ is **ALWAYS** non-decreasing
  - ✔ $ELBO(q^{(n+1)}, \boldsymbol{\theta}^{(n+1)}) \geq ELBO(q^{(n)}, \boldsymbol{\theta}^{(n)})$
  - ✔ Convergence is guaranteed … but to local optimum ...



Initialisation Matters (3)

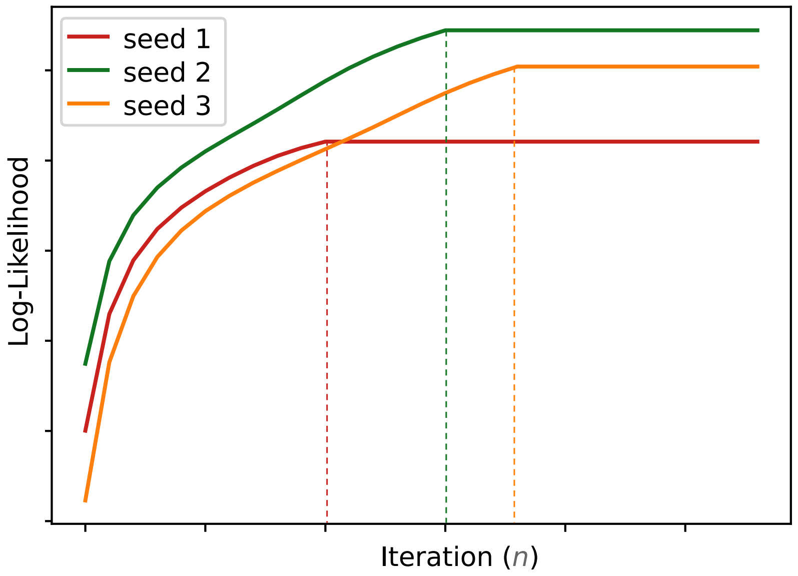
- $p(\mathbf{X}|\theta^{(n)})$ is **ALWAYS** non-decreasing

- Initialisation affects … convergence rate and final log-likelihood



Initialisation Matters (3)

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



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

Other Considerations

- EM is closely related to **Coordinate Ascent** [App B]
  - E-step: fix $\boldsymbol{\theta}$, optimise q
  - M-step: fix q, optimise $\boldsymbol{\theta}$
- 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 $\boldsymbol{\theta}_{ML}$ for probabilistic models with latent var
- **How**: an iterative two-stage (E-step, M-step) procedure
- **Applications**: GMM, HMM, Computational biology, …
- **Assignment**: estimate $\boldsymbol{\theta}_{MAP}$ 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
- Others: blog1 blog2

(B) Coordinate Ascent

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

Procedure:

INITIALISE $\boldsymbol{x}^{(0)} = [x_0, x_1, \ldots, x_{D-1}]$

FOR i in range(#iterations):

FOR d in range(D):

constants

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