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 ...

Maximum Likelihood from Incomplete Data via the *EM* Algorithm

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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

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

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

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

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

Setup

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

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

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

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

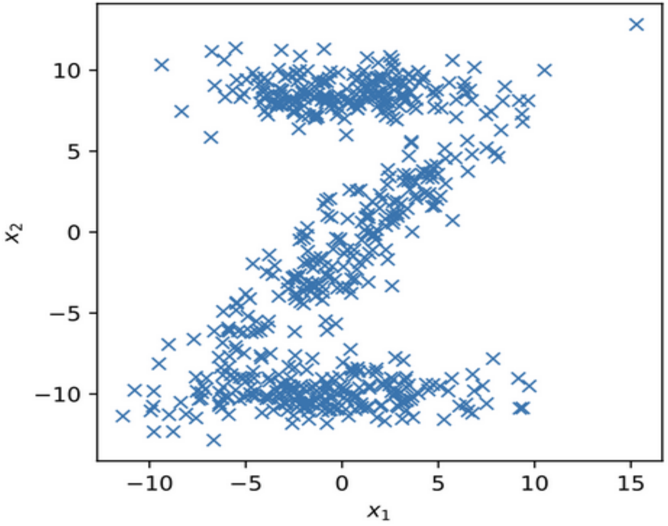
$$= \underset{\theta \in \Theta}{\operatorname{argmax}} \; \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\theta)$$

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

Latent Variable (Z)

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

Incomplete data (X)

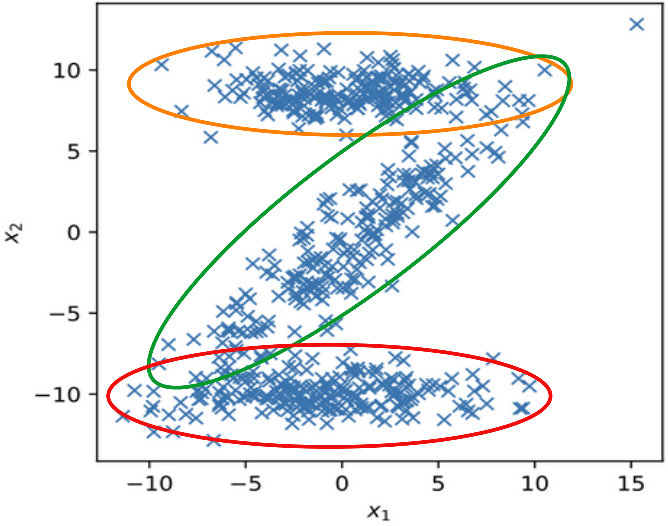


Interpretation: *latent variable* is a part of a model ... *explains **X***.

Latent Variable (Z)

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

Incomplete data (X)



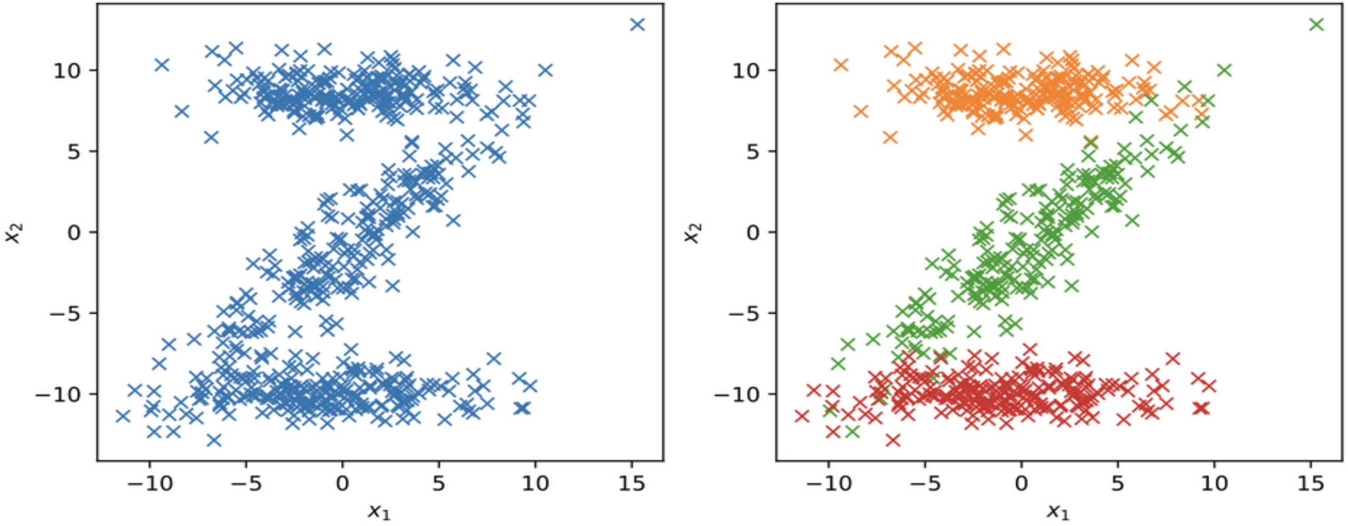
Consider clustering ...

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

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

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

Step 1 Step 2 Step 3

θ_0: derivative roots

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!)

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

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

Step 1 **Step 2** Step 3

θ_0: derivative roots

Direction solution does not work!

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

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!

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

… = 0 → Intractable

Direction solution does not work!

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

$\ldots = 0 \rightarrow$ Intractable

If we could swap log & Σ ...

$\ldots = 0 \rightarrow$ 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*

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

$$\neq$$

Optimise … θ*

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

Intractable

Tractable

(when p belongs to the exponential family)

Optimise … θ^*

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

$\neq$

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

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

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

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

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

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

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

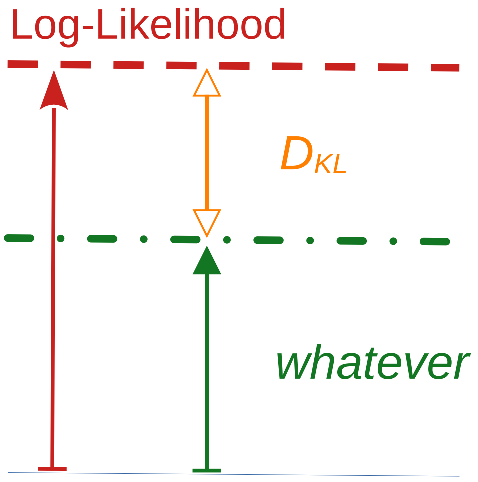
EM Derivation – Step 5.2

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

???

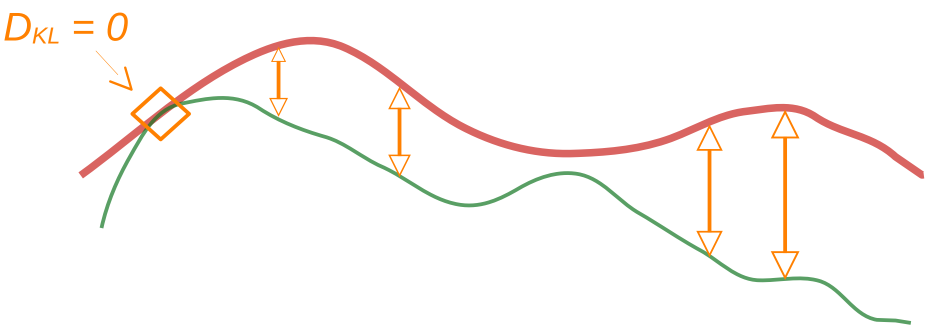
EM Derivation – Step 5.2

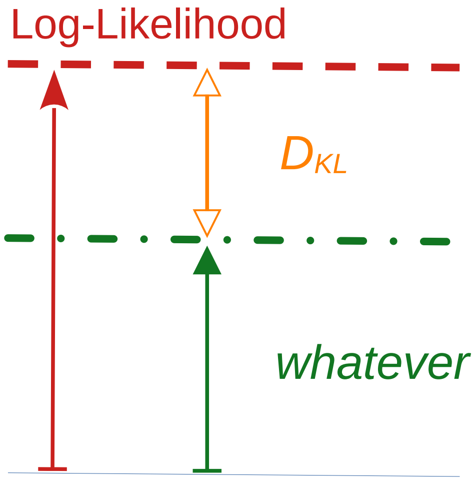
$$\log p(\mathbf{X}|\theta) = \text{whatever} + \underbrace{D_{KL}(q(\mathbf{Z}) \;||\; p(\mathbf{Z}|\mathbf{X},\theta))}_{\geq 0}$$



EM Derivation – Step 5.2

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

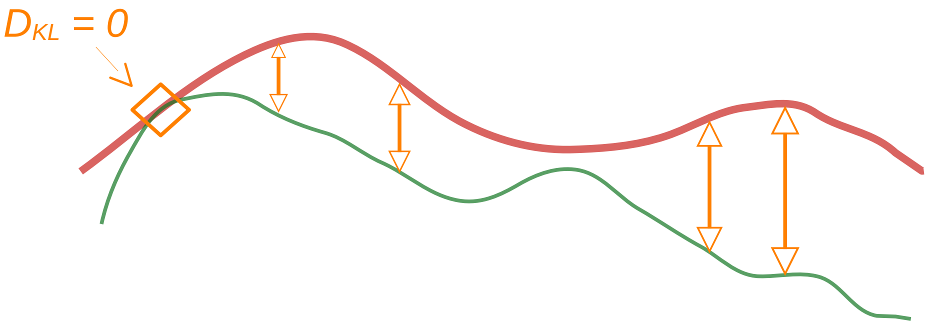


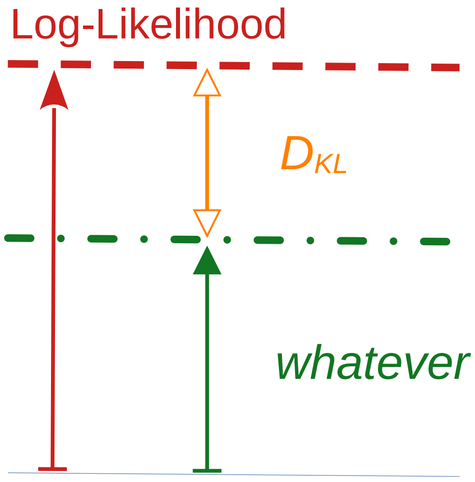


EM Derivation – Step 5.2

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

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





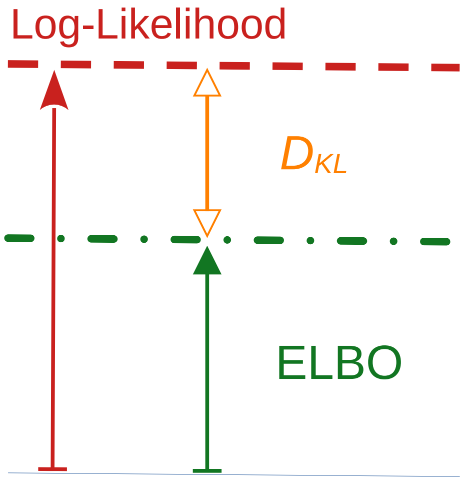
EM Derivation – Step 5.2

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

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

Evidence Lower Bound (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!

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

… = 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

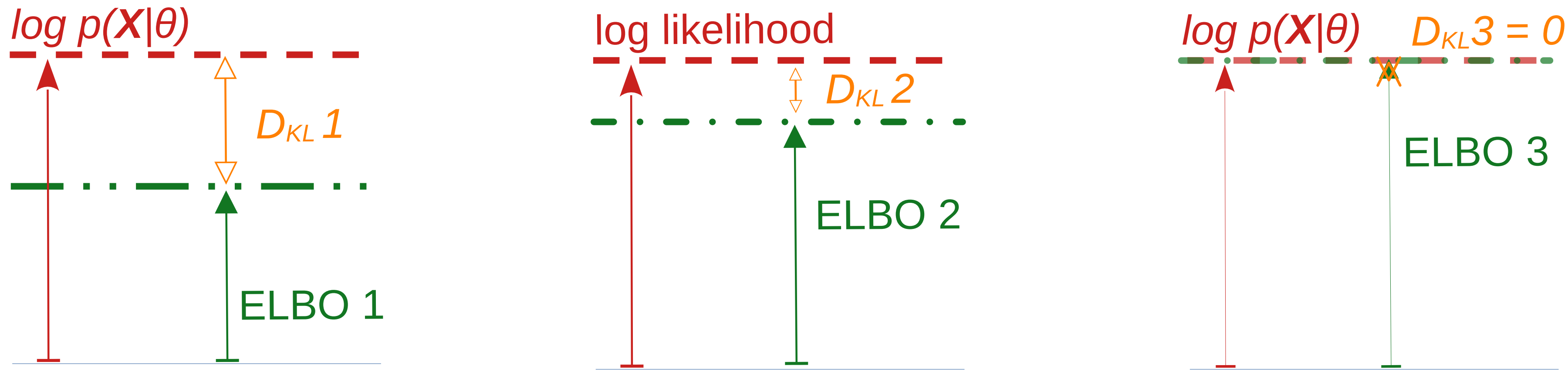
$$\underbrace{\log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z})}_{\log p(\mathbf{X}|\theta)} = \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} \right]}_{ELBO(q,\theta)} + \underbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \left[\frac{q(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{X},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

Tractable

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

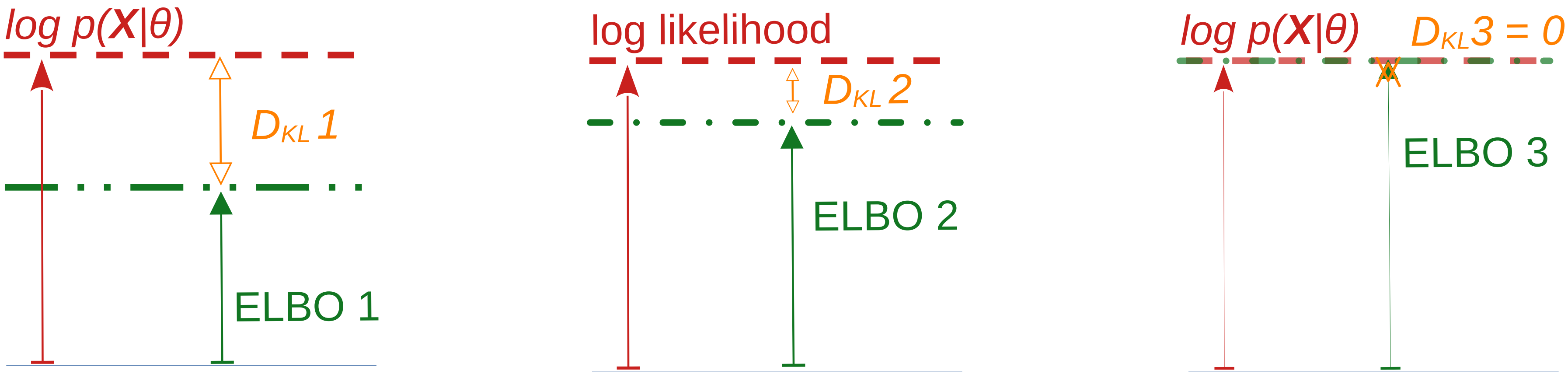
EM $\rightarrow$ Instead of log-likelihood ... maximise ELBO …

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

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

M-step

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

Converged?

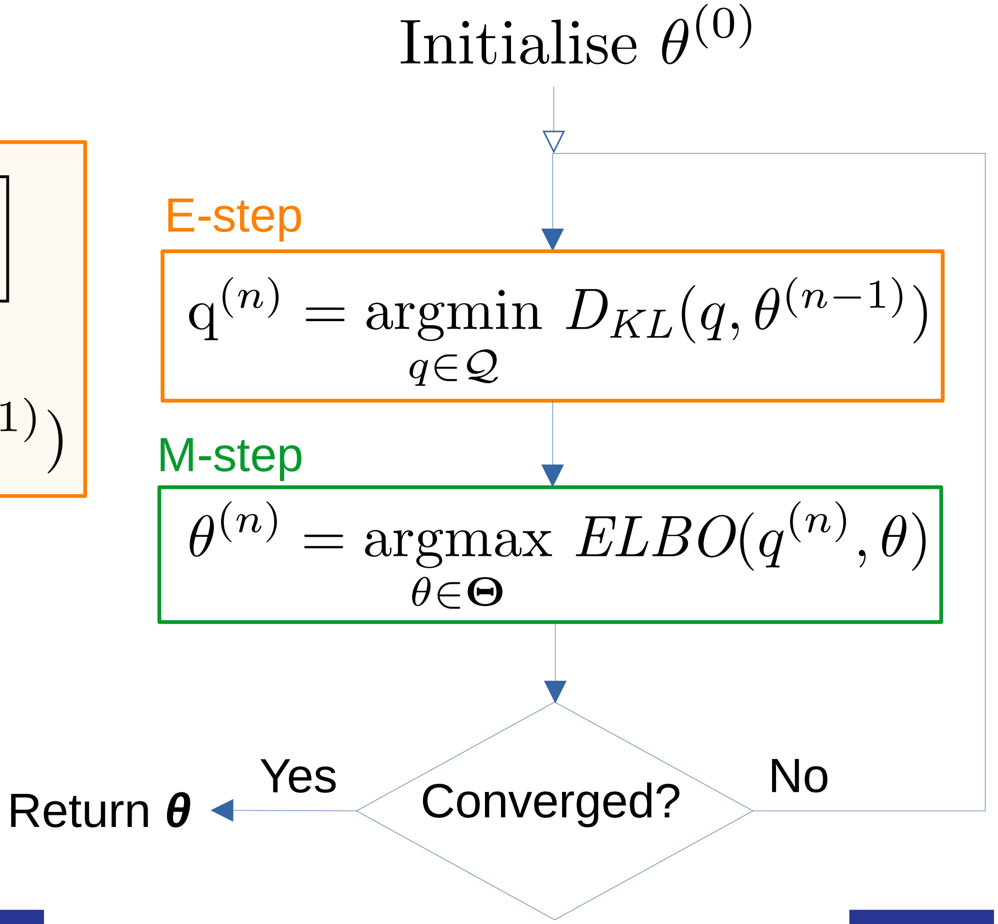
Yes: Return $\boldsymbol{\theta}$

No

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

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

M-Step

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

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

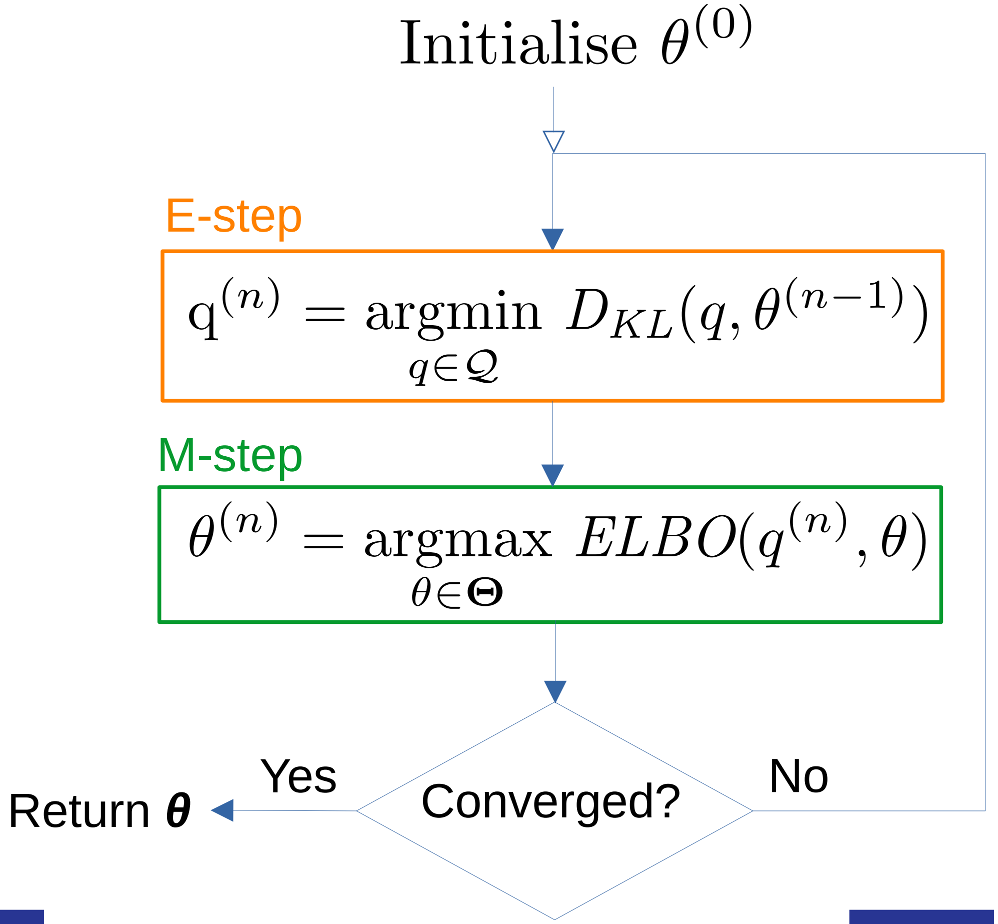
$$\theta^* = \underset{\theta \in \Theta}{\operatorname{argmax}} \; ELBO(q^{(n)}, \theta)$$

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

M-Step

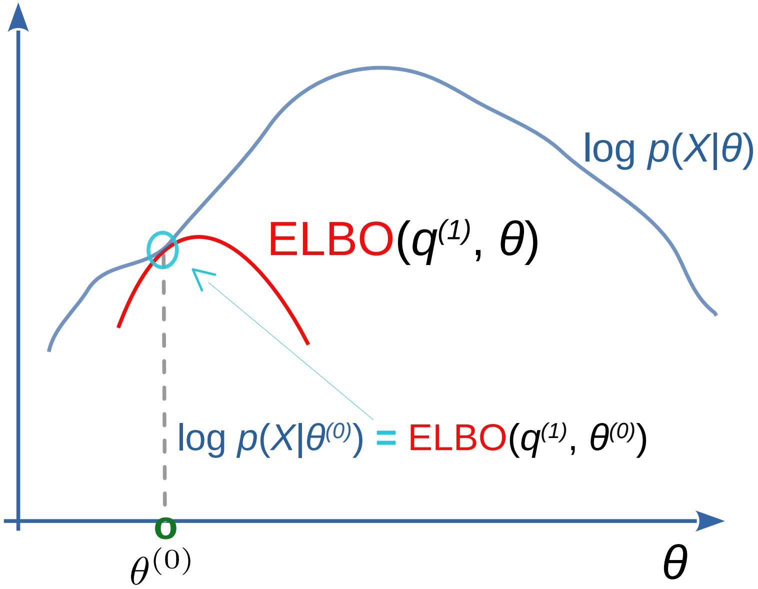
M-step

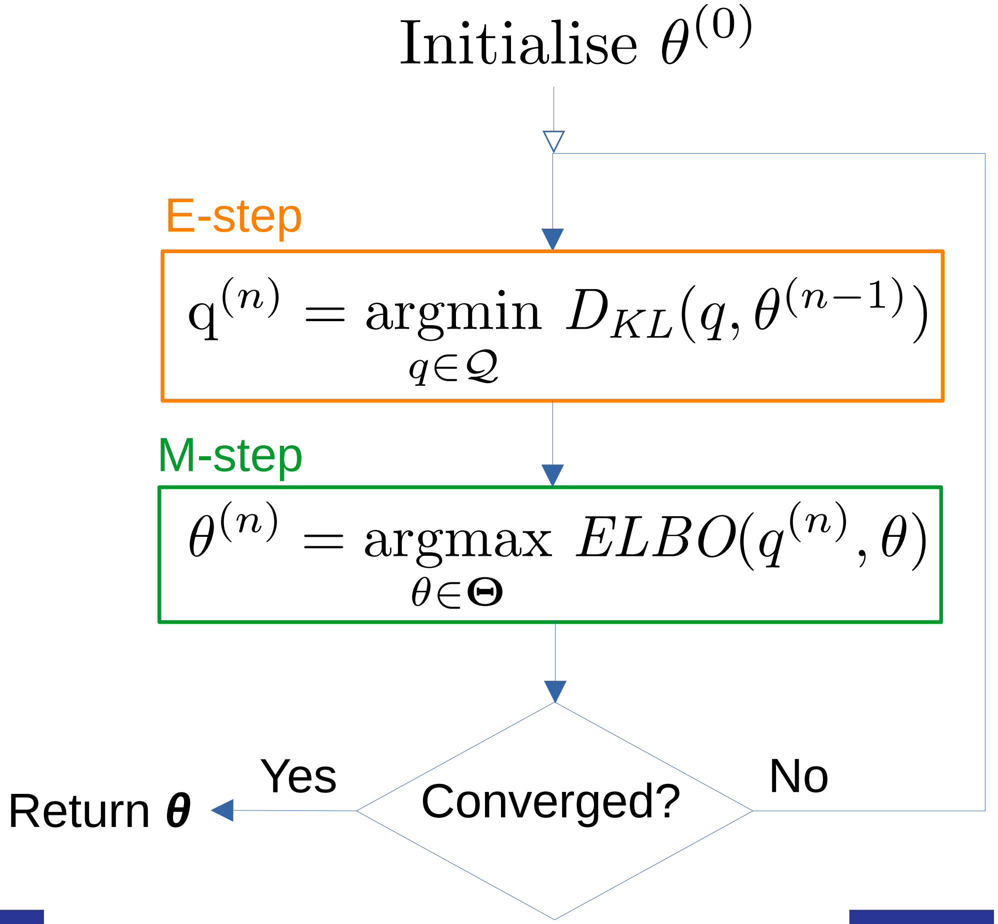
$$\theta^* = \underset{\theta \in \Theta}{\operatorname{argmax}}\; ELBO(q^{(n)}, \theta)$$
$$= \underset{\theta \in \Theta}{\operatorname{argmax}} \sum_{\mathbf{Z}} q^{(n)}(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z} | \theta)$$



Visualisation

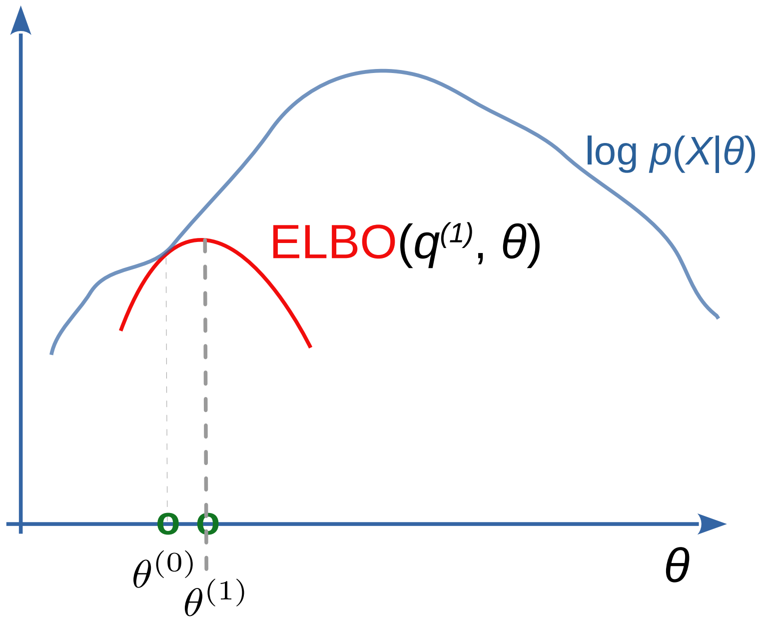
E-step: $q^{(1)} = \text{argmin}\ D_{KL}(q, \theta^{(0)})$

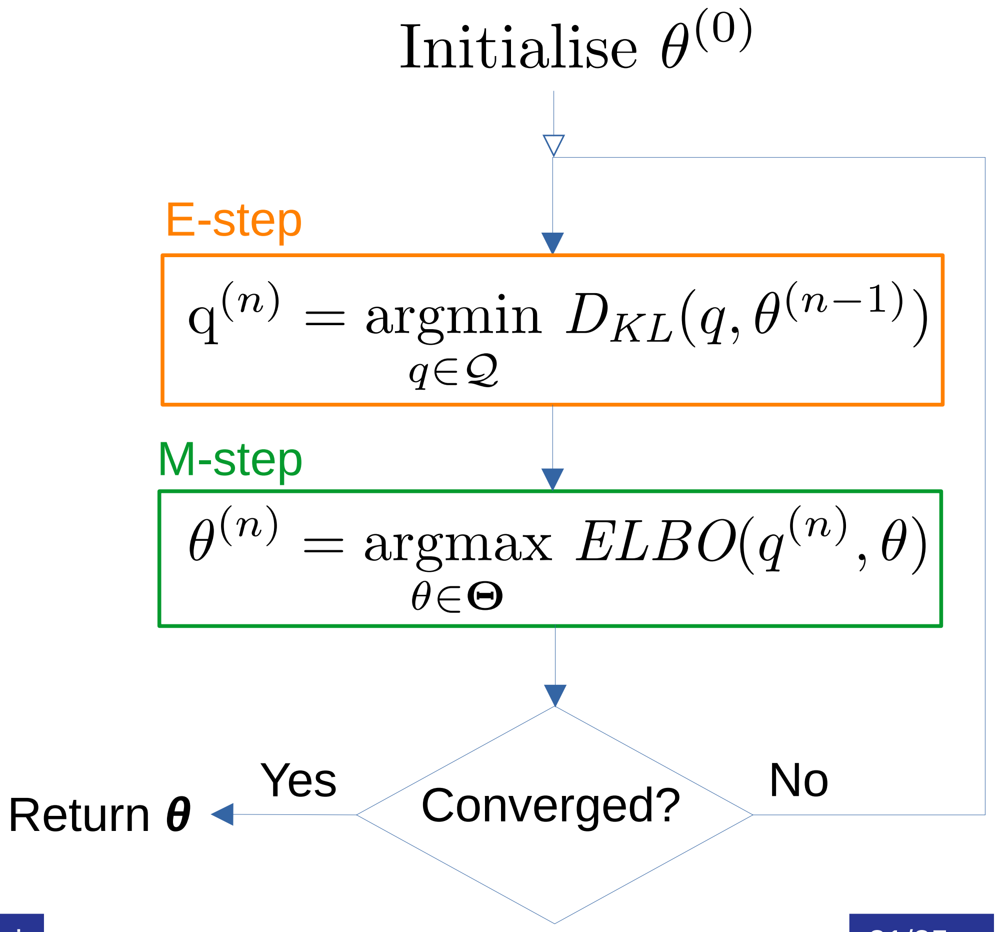




Visualisation

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

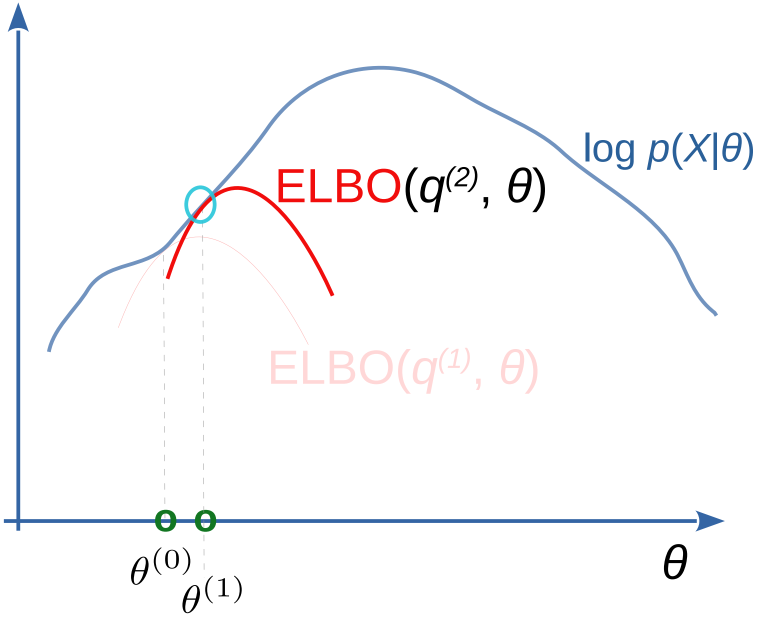


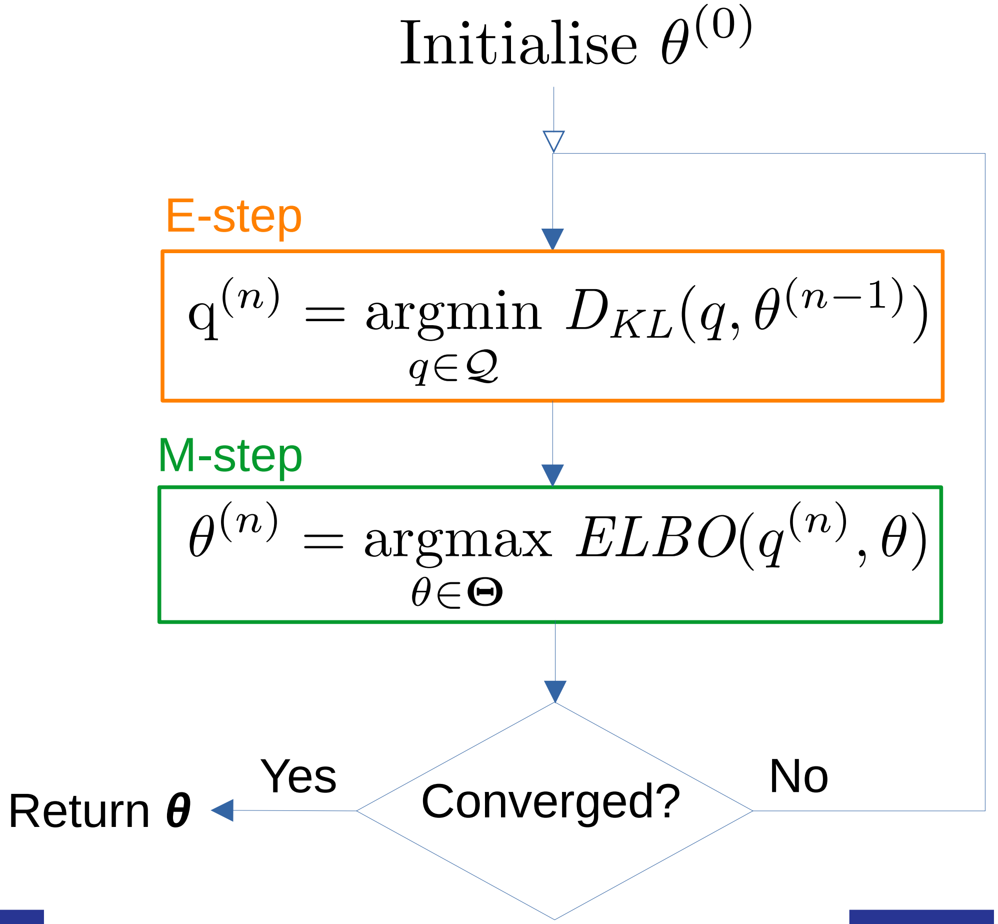


Visualisation

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

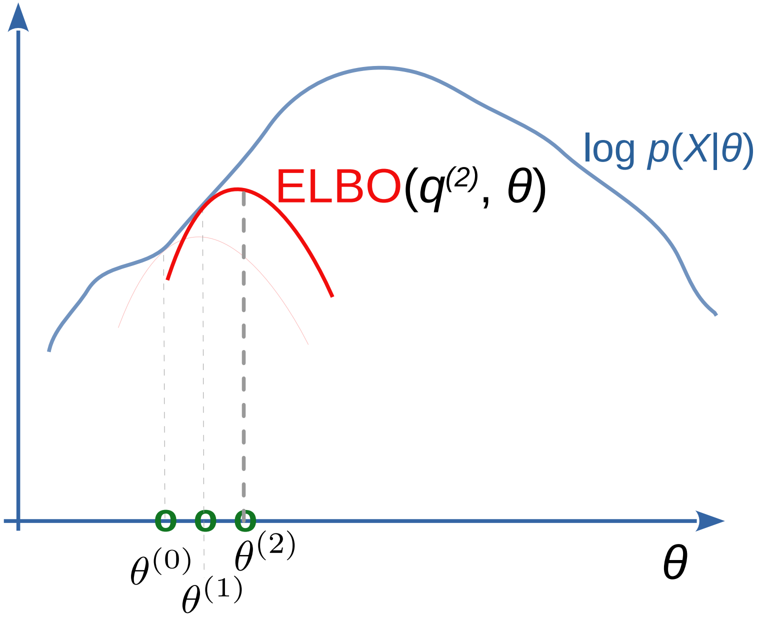
$\log p(X|\theta^{(1)}) = \text{ELBO}(q^{(2)}, \theta^{(1)})$





Visualisation

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



Initialise $\theta^{(0)}$

E-step

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

M-step

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

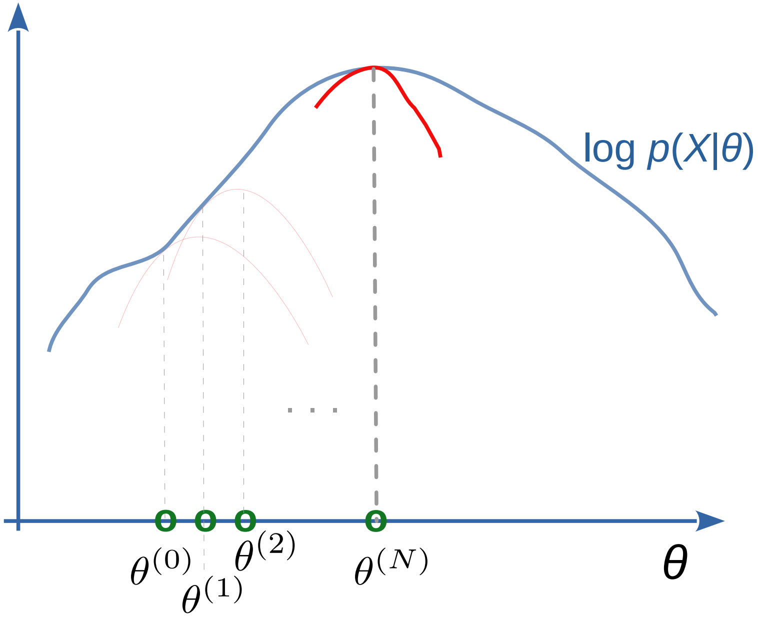
Converged?

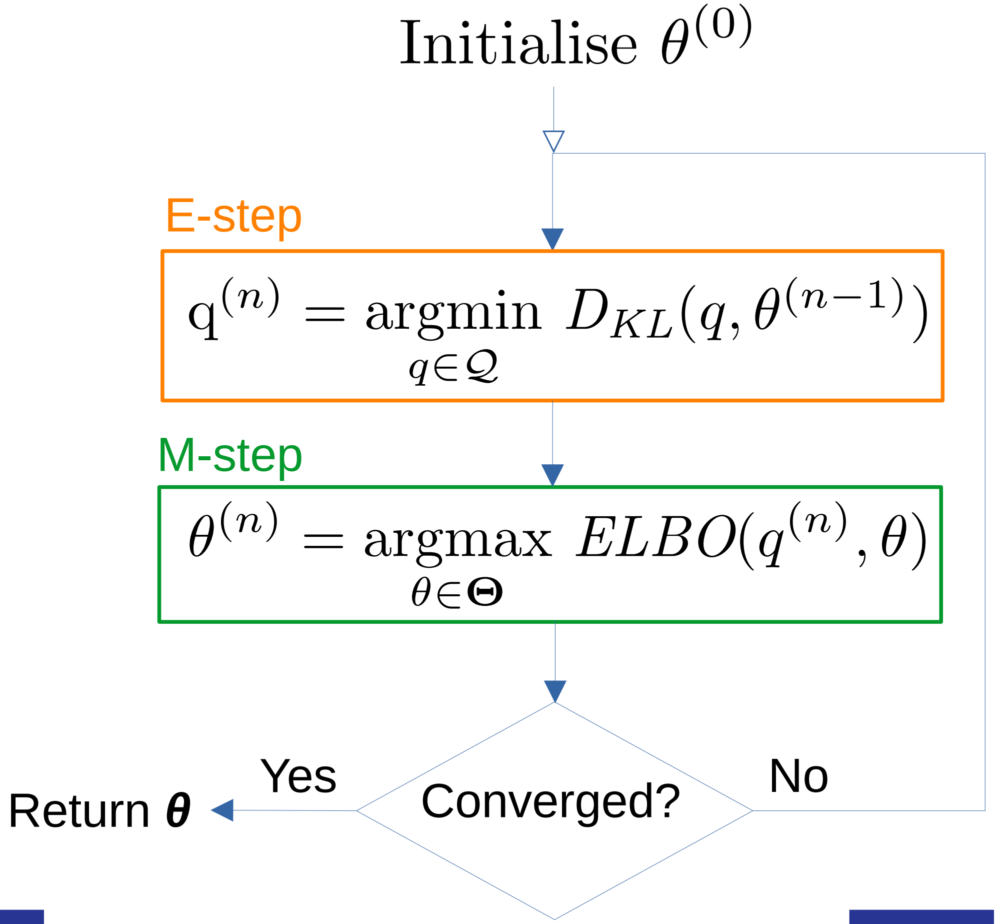
Yes: Return $\boldsymbol{\theta}$

No

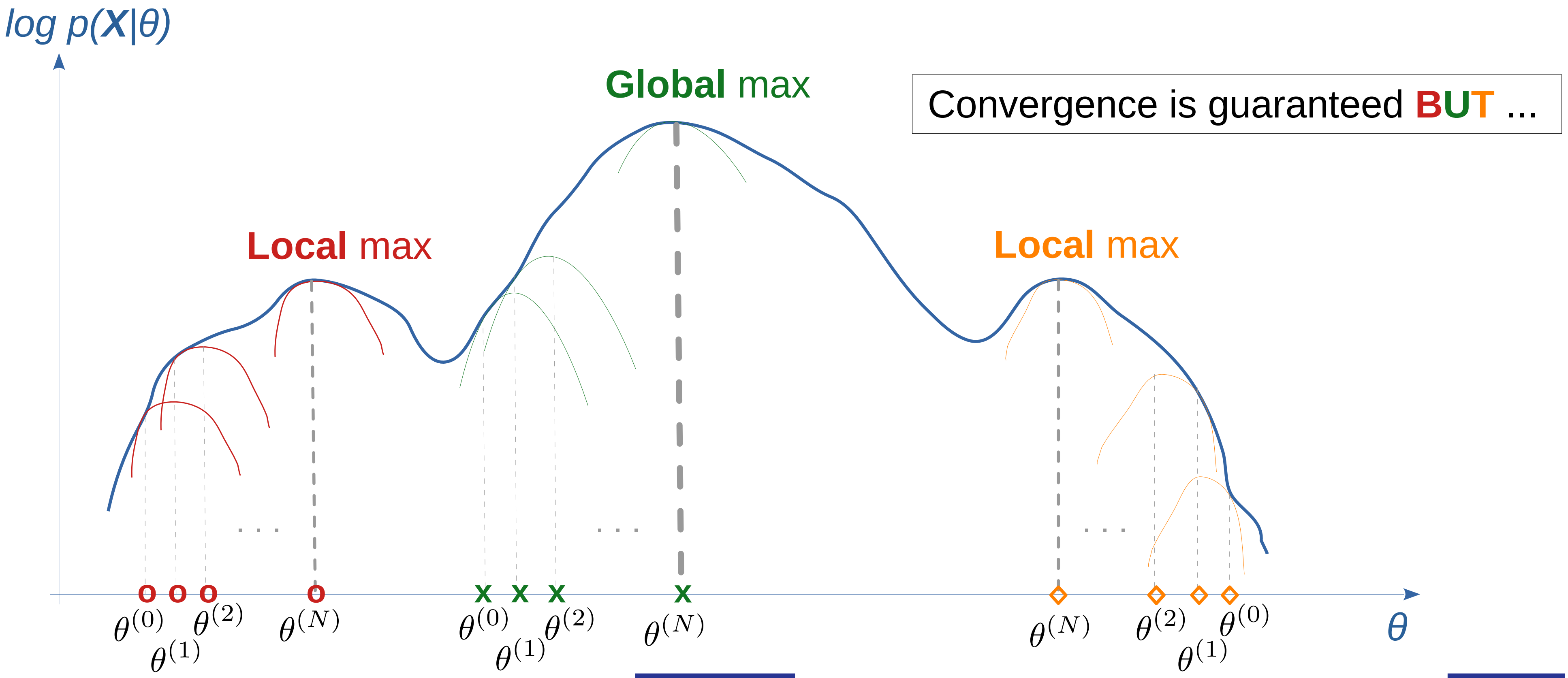
Visualisation

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



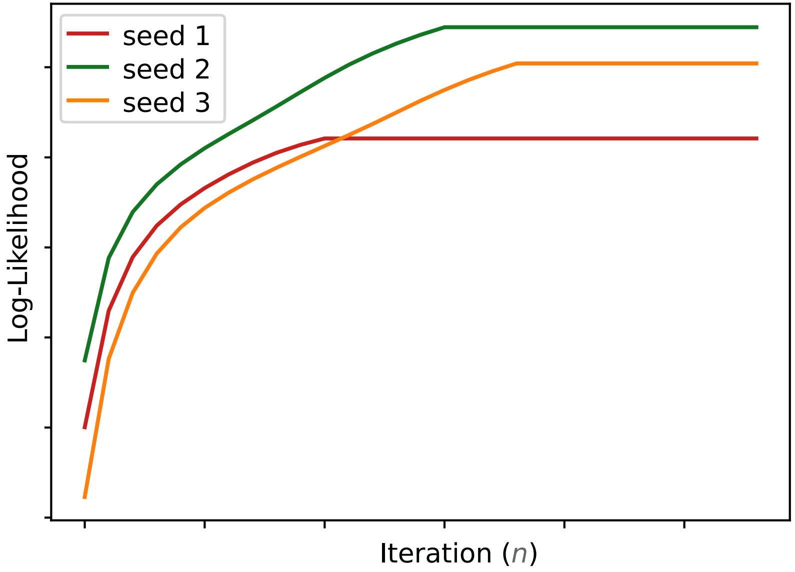


Initialisation Matters (1)



Initialisation Matters (2)

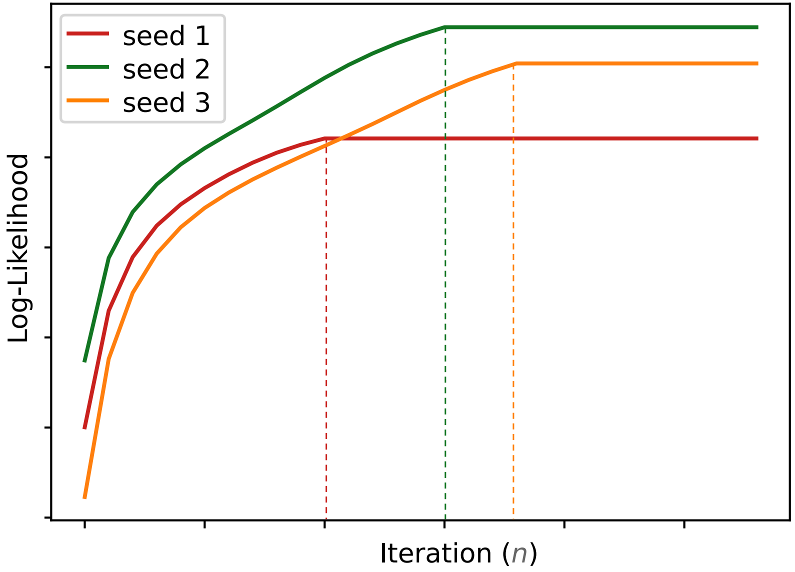
- $p(\mathbf{X}|\theta^{(n)})$ is **ALWAYS** non-decreasing
  - ✓ $ELBO(q^{(n+1)}, \boldsymbol{\theta}^{(n+1)}) \geq ELBO(q^{(n)}, \boldsymbol{\theta}^{(n)})$
  - ✓ Convergence is guaranteed … but to local optimum ...



Initialisation Matters (3)

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

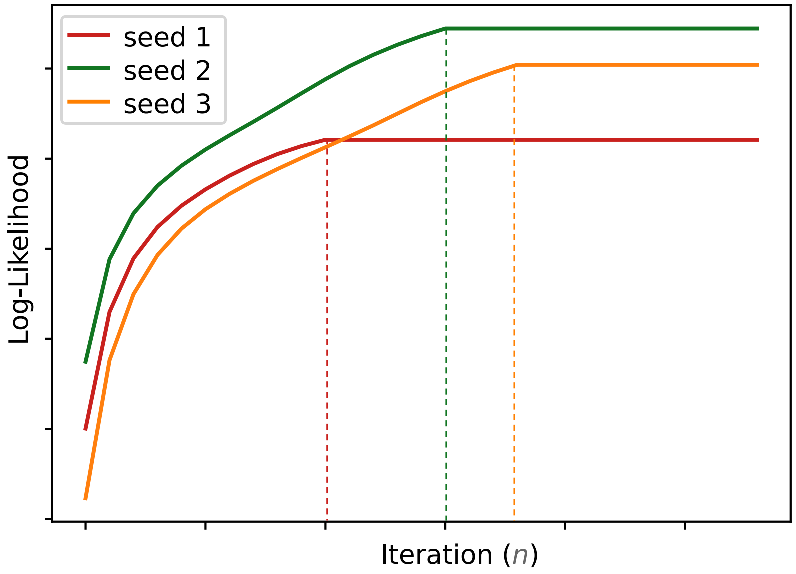
- Initialisation affects … convergence rate and final log-likelihood



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 θ, optimise q
  - M-step: fix q, optimise θ
- EM shines when M-step can be solved analytically
- Alternatives when M-step is intractable ...
  - Generalised EM (**GEM**) $\rightarrow$ (conjugate) gradient ascent in M-Step
  - Expectation Conditional Maximisation (**ECM**) $\rightarrow$ 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

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

<u>axis-aligned movements</u>