Probabilistic & Unsupervised Learning

Expectation Maximisation

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Log-likelihoods

- Exponential family models: $p(\mathbf{x}|\boldsymbol{\theta}) = f(\mathbf{x})e^{\boldsymbol{\theta}^\mathsf{T} \mathbf{T}(\mathbf{x})}/Z(\boldsymbol{\theta})$

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   - Usually no closed form optimum.
   - Often multiple local maxima.
   - Direct numerical optimisation may be possible but infrequently easy.

Example: mixture of Gaussians
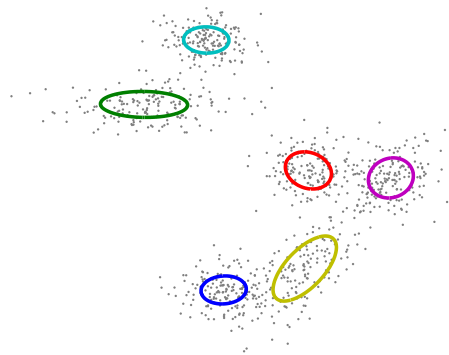
Data: $\mathcal{X} = \{\mathbf{x}_1 \ldots \mathbf{x}_N\}$

Latent process:
$$s_i \overset{\text{iid}}{\sim} \text{Disc}[\boldsymbol{\pi}]$$

Component distributions:
$$\mathbf{x}_i \mid (s_i = m) \sim \mathcal{P}_m[\theta_m] = \mathcal{N}(\boldsymbol{\mu}_m, \boldsymbol{\Sigma}_m)$$

Marginal distribution:
$$P(\mathbf{x}_i) = \sum_{m=1}^{k} \pi_m P_m(\mathbf{x}; \theta_m)$$

Log-likelihood:

$$\ell(\{\boldsymbol{\mu}_m\}, \{\boldsymbol{\Sigma}_m\}, \boldsymbol{\pi}) = \sum_{i=1}^{n} \log \sum_{m=1}^{k} \frac{\pi_m}{\sqrt{|2\pi\boldsymbol{\Sigma}_m|}} e^{-\frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_m)^\mathsf{T} \boldsymbol{\Sigma}_m^{-1}(\mathbf{x}_i - \boldsymbol{\mu}_m)}$$

The joint-data likelihood and EM

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▶ Typically, it will (as we shall see). This is the Expectation Maximisation (EM) algorithm.

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The EM algorithm (Dempster, Laird & Rubin, 1977; but significant earlier precedents) finds a (local) maximum of a latent variable model likelihood.

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▶ Provides a framework for principled approximations.

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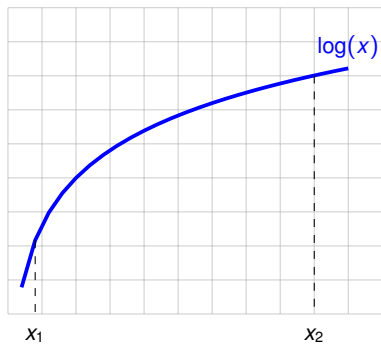
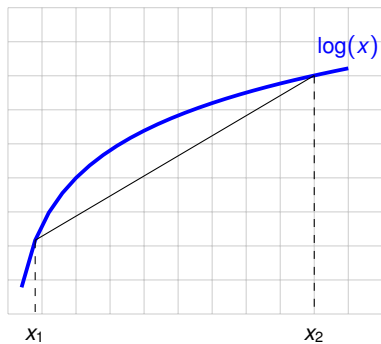# Jensen's inequality

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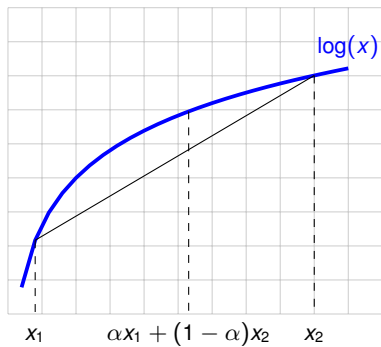One view: EM iteratively refines a lower bound on the log-likelihood.

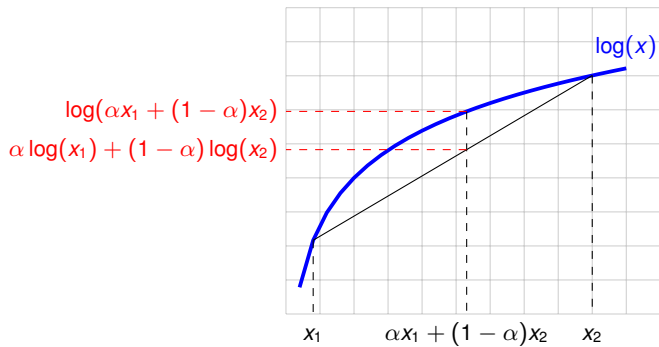# Jensen's inequality

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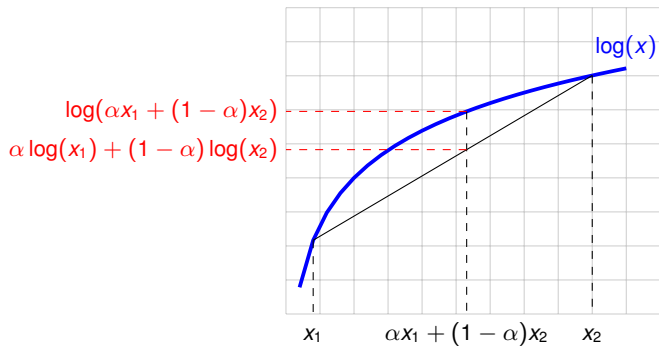
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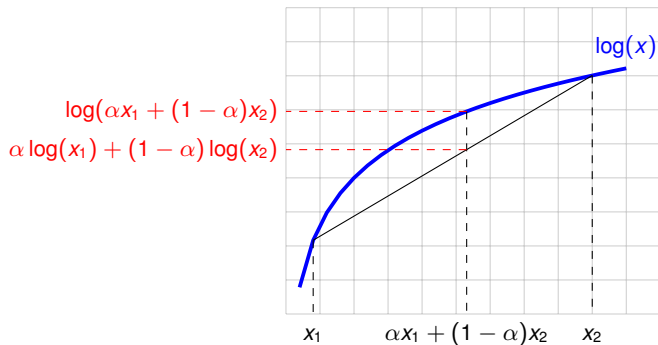
In general:

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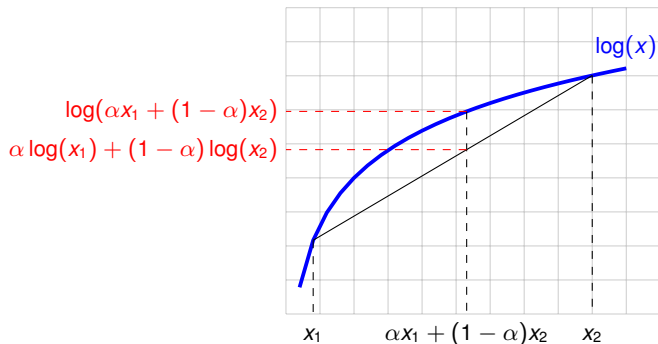
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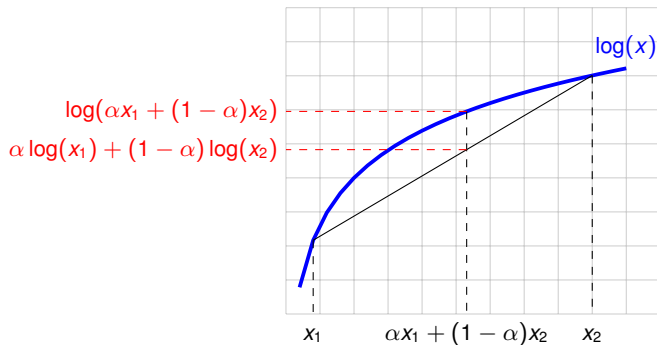
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Equality (if and) only if $f(x)$ is almost surely constant or linear on (convex) support of α.

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So:
$$\mathcal{F}(q, \theta) = \langle \log P(\mathcal{Z}, \mathcal{X}|\theta) \rangle_{q(\mathcal{Z})} + \mathbf{H}[q]$$

The E and M steps of EM

The free-energy lower bound on $\ell(\theta)$ is a function of θ and a distribution q:

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The second equality comes from the fact that $\mathbf{H}\Big[q^{(k)}(\mathcal{Z})\Big]$ does not depend directly on θ.

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$$
\begin{aligned}
\mathcal{F}(q, \theta) &= \int q(\mathcal{Z}) \log \frac{P(\mathcal{Z}, \mathcal{X}|\theta)}{q(\mathcal{Z})} \, d\mathcal{Z} \\
&= \int q(\mathcal{Z}) \log \frac{P(\mathcal{Z}|\mathcal{X}, \theta)P(\mathcal{X}|\theta)}{q(\mathcal{Z})} \, d\mathcal{Z} \\
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The second term is the Kullback-Leibler divergence.

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This means that, for fixed θ, $\mathcal{F}$ is bounded above by ℓ, and achieves that bound when $\textbf{KL}[q(\mathcal{Z}) \| P(\mathcal{Z}|\mathcal{X}, \theta)] = 0$.

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But $\mathbf{KL}[q \| p]$ is zero if and only if $q = p$ (see appendix.)

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But $\mathbf{KL}[q\|p]$ is zero if and only if $q = p$ (see appendix.)

So, the E step sets

$$q^{(k)}(\mathcal{Z}) = P(\mathcal{Z}|\mathcal{X}, \theta^{(k-1)}) \qquad \text{[inference / imputation]}$$

and, after an E step, the free energy equals the likelihood.

Coordinate Ascent in $\mathcal{F}$ (Demo)

To visualise, we consider a one parameter / one latent mixture:

$$s \sim \text{Bernoulli}[\pi]$$
$$x|s = 0 \sim \mathcal{N}[-1, 1] \qquad x|s = 1 \sim \mathcal{N}[1, 1].$$

Single data point $x_1 = .3$.
$q(s)$ is a distribution on a single binary latent, and so is represented by $r_1 \in [0, 1]$.

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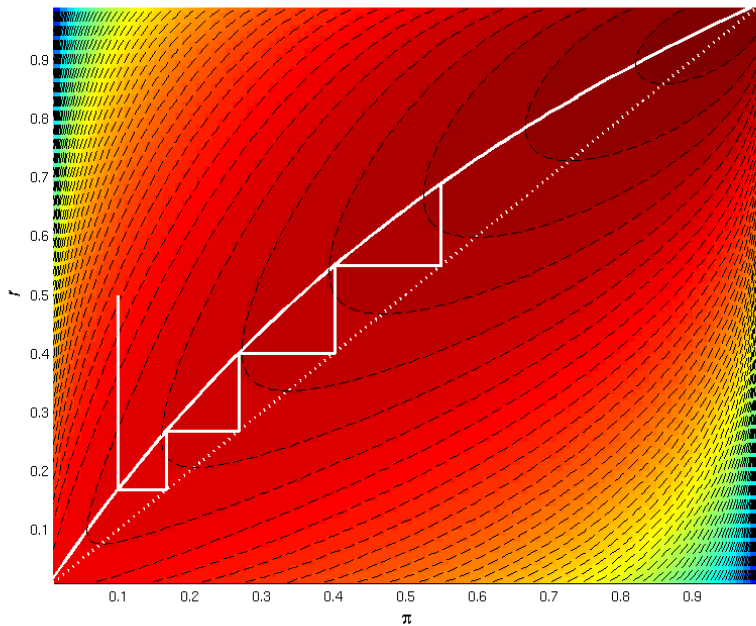
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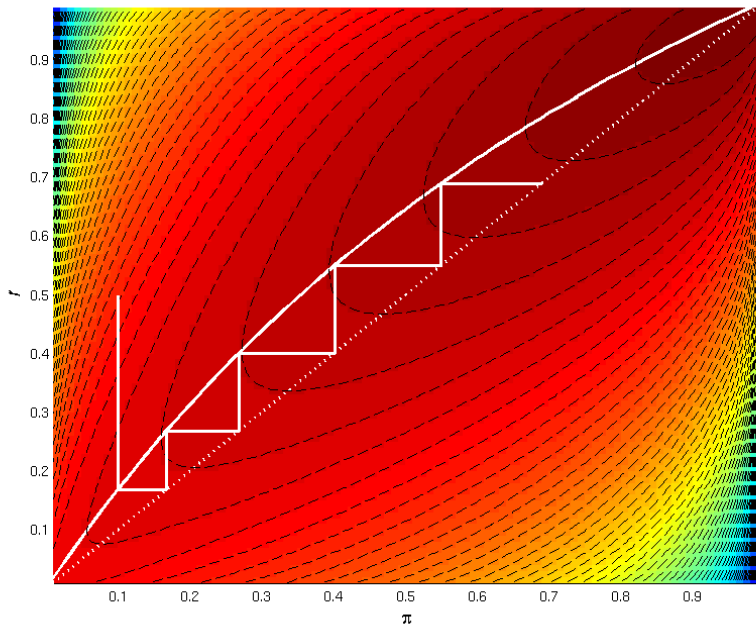
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EM Never Decreases the Likelihood

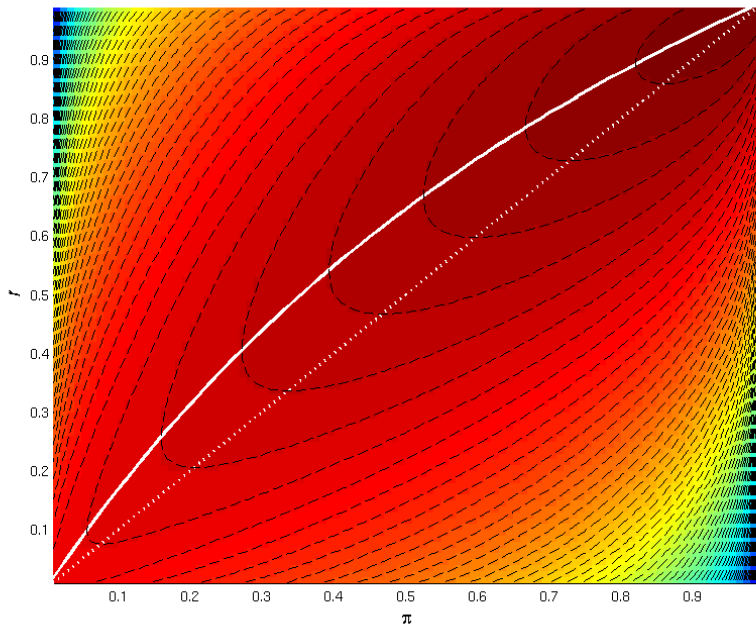The E and M steps together never decrease the log likelihood:

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If the M-step is executed so that $\theta^{(k)} \neq \theta^{(k-1)}$ iff $\mathcal{F}$ increases, then the overall EM iteration will step to a new value of θ iff the likelihood increases.

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Can also show that fixed points of EM (generally) correspond to maxima of the likelihood (see appendices).

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▶ An iterative algorithm that finds (local) maxima of the likelihood of a latent variable model.

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▶ After E-step $\mathcal{F}(q, \theta) = \ell(\theta) \Rightarrow$ maximum of free-energy is maximum of likelihood.

Partial M steps and Partial E steps

Partial M steps: The proof holds even if we just *increase* $\mathcal{F}$ wrt θ rather than maximize. (Dempster, Laird and Rubin (1977) call this the generalized EM, or GEM, algorithm).

In fact, immediately after an E step

$$\frac{\partial}{\partial\theta}\bigg|_{\theta^{(k-1)}} \langle \log P(\mathcal{X}, \mathcal{Z}|\theta)\rangle_{q^{(k)}(\mathcal{Z})[=P(\mathcal{Z}|\mathcal{X},\theta^{(k-1)})]} = \frac{\partial}{\partial\theta}\bigg|_{\theta^{(k-1)}} \log P(\mathcal{X}|\theta)$$

[cf. mixture gradients from last lecture.] So E-step (inference) can be used to construct other gradient-based optimisation schemes (e.g. "Expectation Conjugate Gradient", Salakhutdinov et al. *ICML* 2003).

Partial E steps: We can also just *increase* $\mathcal{F}$ wrt to some of the qs.

For example, sparse or online versions of the EM algorithm would compute the posterior for a subset of the data points or as the data arrives, respectively. One might also update the posterior over a subset of the hidden variables, while holding others fixed...

EM for MoGs
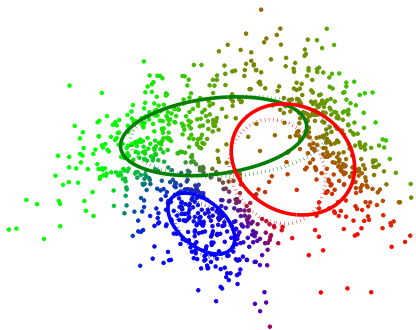
▶ Evaluate responsibilities

$$r_{im} = \frac{P_m(\mathbf{x})\pi_m}{\sum_{m'} P_{m'}(\mathbf{x})\pi_{m'}}$$

▶ Update parameters

$$\boldsymbol{\mu}_m \leftarrow \frac{\sum_i r_{im}\mathbf{x}_i}{\sum_i r_{im}}$$

$$\boldsymbol{\Sigma}_m \leftarrow \frac{\sum_i r_{im}(\mathbf{x}_i - \boldsymbol{\mu}_m)(\mathbf{x}_i - \boldsymbol{\mu}_m)^\mathsf{T}}{\sum_i r_{im}}$$

$$\pi_m \leftarrow \frac{\sum_i r_{im}}{N}$$

The Gaussian mixture model (E-step)

In a univariate Gaussian mixture model, the density of a data point x is:

$$p(x|\theta) = \sum_{m=1}^{k} p(s = m|\theta)p(x|s = m, \theta) \propto \sum_{m=1}^{k} \frac{\pi_m}{\sigma_m} \exp\left\{ -\frac{1}{2\sigma_m^2}(x - \mu_m)^2 \right\},$$

where θ is the collection of parameters: means μ_m, variances σ_m^2 and mixing proportions $\pi_m = p(s = m|\theta)$.

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In the M-step we optimize the sum (since s is discrete):

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$$\frac{\partial}{\partial \sigma_m} E = \sum_i r_{im} \Big[-\frac{1}{\sigma_m} + \frac{(x_i - \mu_m)^2}{\sigma_m^3} \Big] = 0 \;\; \Rightarrow \;\; \sigma_m^2 = \frac{\sum_i r_{im}(x_i - \mu_m)^2}{\sum_i r_{im}},$$

$$\frac{\partial}{\partial \pi_m} E = \sum_i r_{im} \frac{1}{\pi_m}, \qquad \frac{\partial E}{\partial \pi_m} + \lambda = 0 \;\; \Rightarrow \;\; \pi_m = \frac{1}{n} \sum_i r_{im},$$

where λ is a Lagrange multiplier ensuring that the mixing proportions sum to unity.

EM for Factor Analysis
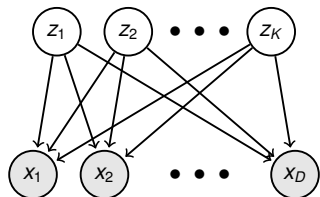
The model for **x**:

$$p(\mathbf{x}|\theta) = \int p(\mathbf{z}|\theta)p(\mathbf{x}|\mathbf{z}, \theta)d\mathbf{z} = \mathcal{N}(0, \Lambda\Lambda^{\mathsf{T}} + \Psi)$$

Model parameters: $\theta = \{\Lambda, \Psi\}$.

E step: For each data point $\mathbf{x}_n$, compute the posterior distribution of hidden factors given the observed data: $q_n(\mathbf{z}_n) = p(\mathbf{z}_n|\mathbf{x}_n, \theta_t)$.

M step: Find the θ_{t+1} that maximises $\mathcal{F}(q, \theta)$:

$$
\begin{aligned}
\mathcal{F}(q, \theta) &= \sum_n \int q_n(\mathbf{z}_n) \left[\log p(\mathbf{z}_n|\theta) + \log p(\mathbf{x}_n|\mathbf{z}_n, \theta) - \log q_n(\mathbf{z}_n)\right] d\mathbf{z}_n \\
&= \sum_n \int q_n(\mathbf{z}_n) \left[\log p(\mathbf{z}_n|\theta) + \log p(\mathbf{x}_n|\mathbf{z}_n, \theta)\right] d\mathbf{z}_n + \mathrm{c}.
\end{aligned}
$$

The E step for Factor Analysis

E step: For each data point $\mathbf{x}_n$, compute the posterior distribution of hidden factors given the observed data: $q_n(\mathbf{z}_n) = p(\mathbf{z}_n|\mathbf{x}_n, \theta) = p(\mathbf{z}_n, \mathbf{x}_n|\theta)/p(\mathbf{x}_n|\theta)$

Tactic: write $p(\mathbf{z}_n, \mathbf{x}_n|\theta)$, consider $\mathbf{x}_n$ to be fixed. What is this as a function of $\mathbf{z}_n$?

$$
\begin{aligned}
p(\mathbf{z}_n, \mathbf{x}_n) &= p(\mathbf{z}_n)p(\mathbf{x}_n|\mathbf{z}_n) \\
&= (2\pi)^{-\frac{K}{2}} \exp\{-\frac{1}{2}\mathbf{z}_n^\mathsf{T}\mathbf{z}_n\} \, |2\pi\Psi|^{-\frac{1}{2}} \exp\{-\frac{1}{2}(\mathbf{x}_n - \Lambda\mathbf{z}_n)^\mathsf{T}\Psi^{-1}(\mathbf{x}_n - \Lambda\mathbf{z}_n)\} \\
&= c \times \exp\{-\frac{1}{2}[\mathbf{z}_n^\mathsf{T}\mathbf{z}_n + (\mathbf{x}_n - \Lambda\mathbf{z}_n)^\mathsf{T}\Psi^{-1}(\mathbf{x}_n - \Lambda\mathbf{z}_n)]\} \\
&= c' \times \exp\{-\frac{1}{2}[\mathbf{z}_n^\mathsf{T}(I + \Lambda^\mathsf{T}\Psi^{-1}\Lambda)\mathbf{z}_n - 2\mathbf{z}_n^\mathsf{T}\Lambda^\mathsf{T}\Psi^{-1}\mathbf{x}_n]\} \\
&= c'' \times \exp\{-\frac{1}{2}[\mathbf{z}_n^\mathsf{T}\Sigma^{-1}\mathbf{z}_n - 2\mathbf{z}_n^\mathsf{T}\Sigma^{-1}\boldsymbol{\mu}_n + \boldsymbol{\mu}_n^\mathsf{T}\Sigma^{-1}\boldsymbol{\mu}_n]\}
\end{aligned}
$$

So $\Sigma = (I + \Lambda^\mathsf{T}\Psi^{-1}\Lambda)^{-1} = I - \beta\Lambda$ and $\boldsymbol{\mu}_n = \Sigma\Lambda^\mathsf{T}\Psi^{-1}\mathbf{x}_n = \beta\mathbf{x}_n$. Where $\beta = \Sigma\Lambda^\mathsf{T}\Psi^{-1}$. Note that $\boldsymbol{\mu}_n$ is a linear function of $\mathbf{x}_n$ and Σ does not depend on $\mathbf{x}_n$.

The M step for Factor Analysis

M step: Find θ_{t+1} by maximising $\mathcal{F} = \sum_n \langle \log p(\mathbf{z}_n | \theta) + \log p(\mathbf{x}_n | \mathbf{z}_n, \theta) \rangle_{q_n(\mathbf{z}_n)} + c$

The M step for Factor Analysis

M step: Find θ_{t+1} by maximising $\mathcal{F} = \sum_n \langle \log p(\mathbf{z}_n|\theta) + \log p(\mathbf{x}_n|\mathbf{z}_n, \theta) \rangle_{q_n(\mathbf{z}_n)} + c$

$\log p(\mathbf{z}_n|\theta) + \log p(\mathbf{x}_n|\mathbf{z}_n, \theta)$

The M step for Factor Analysis

M step: Find θ_{t+1} by maximising $\mathcal{F} = \sum_n \langle \log p(\mathbf{z}_n|\theta) + \log p(\mathbf{x}_n|\mathbf{z}_n, \theta) \rangle_{q_n(\mathbf{z}_n)} + c$

$\log p(\mathbf{z}_n|\theta) + \log p(\mathbf{x}_n|\mathbf{z}_n, \theta)$

$= c - \frac{1}{2}\mathbf{z}_n^\mathsf{T}\mathbf{z}_n - \frac{1}{2}\log|\Psi| - \frac{1}{2}(\mathbf{x}_n - \Lambda\mathbf{z}_n)^\mathsf{T}\Psi^{-1}(\mathbf{x}_n - \Lambda\mathbf{z}_n)$

The M step for Factor Analysis

M step: Find θ_{t+1} by maximising $\mathcal{F} = \sum_n \langle \log p(\mathbf{z}_n|\theta) + \log p(\mathbf{x}_n|\mathbf{z}_n, \theta) \rangle_{q_n(\mathbf{z}_n)} + c$

$$\log p(\mathbf{z}_n|\theta) + \log p(\mathbf{x}_n|\mathbf{z}_n, \theta)$$

$$= c - \frac{1}{2}\mathbf{z}_n^\mathsf{T}\mathbf{z}_n - \frac{1}{2}\log|\Psi| - \frac{1}{2}(\mathbf{x}_n - \Lambda\mathbf{z}_n)^\mathsf{T}\Psi^{-1}(\mathbf{x}_n - \Lambda\mathbf{z}_n)$$

$$= c' - \frac{1}{2}\log|\Psi| - \frac{1}{2}\left[\mathbf{x}_n^\mathsf{T}\Psi^{-1}\mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n + \mathbf{z}_n^\mathsf{T}\Lambda^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n\right]$$

The M step for Factor Analysis

M step: Find θ_{t+1} by maximising $\mathcal{F} = \sum\limits_{n} \left\langle \log p(\mathbf{z}_n|\theta) + \log p(\mathbf{x}_n|\mathbf{z}_n, \theta) \right\rangle_{q_n(\mathbf{z}_n)} + \mathsf{c}$

$$
\begin{aligned}
&\log p(\mathbf{z}_n|\theta) + \log p(\mathbf{x}_n|\mathbf{z}_n, \theta) \\
&= \mathsf{c} - \frac{1}{2}\mathbf{z}_n^\mathsf{T}\mathbf{z}_n - \frac{1}{2}\log|\Psi| - \frac{1}{2}(\mathbf{x}_n - \Lambda\mathbf{z}_n)^\mathsf{T}\Psi^{-1}(\mathbf{x}_n - \Lambda\mathbf{z}_n) \\
&= \mathsf{c'} - \frac{1}{2}\log|\Psi| - \frac{1}{2}\left[\mathbf{x}_n^\mathsf{T}\Psi^{-1}\mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n + \mathbf{z}_n^\mathsf{T}\Lambda^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n\right] \\
&= \mathsf{c'} - \frac{1}{2}\log|\Psi| - \frac{1}{2}\left[\mathbf{x}_n^\mathsf{T}\Psi^{-1}\mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n + \mathsf{Tr}\left[\Lambda^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n\mathbf{z}_n^\mathsf{T}\right]\right]
\end{aligned}
$$

The M step for Factor Analysis

M step: Find θ_{t+1} by maximising $\mathcal{F} = \sum_n \langle \log p(\mathbf{z}_n|\theta) + \log p(\mathbf{x}_n|\mathbf{z}_n, \theta) \rangle_{q_n(\mathbf{z}_n)} + c$

$$\log p(\mathbf{z}_n|\theta) + \log p(\mathbf{x}_n|\mathbf{z}_n, \theta)$$

$$= c - \frac{1}{2}\mathbf{z}_n^\mathsf{T}\mathbf{z}_n - \frac{1}{2}\log|\Psi| - \frac{1}{2}(\mathbf{x}_n - \Lambda\mathbf{z}_n)^\mathsf{T}\Psi^{-1}(\mathbf{x}_n - \Lambda\mathbf{z}_n)$$

$$= c' - \frac{1}{2}\log|\Psi| - \frac{1}{2}\left[\mathbf{x}_n^\mathsf{T}\Psi^{-1}\mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n + \mathbf{z}_n^\mathsf{T}\Lambda^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n\right]$$

$$= c' - \frac{1}{2}\log|\Psi| - \frac{1}{2}\left[\mathbf{x}_n^\mathsf{T}\Psi^{-1}\mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n + \mathrm{Tr}\left[\Lambda^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n\mathbf{z}_n^\mathsf{T}\right]\right]$$

Taking expectations wrt $q_n(\mathbf{z}_n)$:

The M step for Factor Analysis

M step: Find θ_{t+1} by maximising $\mathcal{F} = \sum_n \langle \log p(\mathbf{z}_n|\theta) + \log p(\mathbf{x}_n|\mathbf{z}_n, \theta) \rangle_{q_n(\mathbf{z}_n)} + c$

$\log p(\mathbf{z}_n|\theta) + \log p(\mathbf{x}_n|\mathbf{z}_n, \theta)$

$$= c - \frac{1}{2}\mathbf{z}_n^\mathsf{T}\mathbf{z}_n - \frac{1}{2}\log|\Psi| - \frac{1}{2}(\mathbf{x}_n - \Lambda\mathbf{z}_n)^\mathsf{T}\Psi^{-1}(\mathbf{x}_n - \Lambda\mathbf{z}_n)$$

$$= c' - \frac{1}{2}\log|\Psi| - \frac{1}{2}\left[\mathbf{x}_n^\mathsf{T}\Psi^{-1}\mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n + \mathbf{z}_n^\mathsf{T}\Lambda^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n\right]$$

$$= c' - \frac{1}{2}\log|\Psi| - \frac{1}{2}\left[\mathbf{x}_n^\mathsf{T}\Psi^{-1}\mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n + \mathrm{Tr}\left[\Lambda^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n\mathbf{z}_n^\mathsf{T}\right]\right]$$

Taking expectations wrt $q_n(\mathbf{z}_n)$:

$$= c' - \frac{1}{2}\log|\Psi| - \frac{1}{2}\left[\mathbf{x}_n^\mathsf{T}\Psi^{-1}\mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T}\Psi^{-1}\Lambda\boldsymbol{\mu}_n + \mathrm{Tr}\left[\Lambda^\mathsf{T}\Psi^{-1}\Lambda(\boldsymbol{\mu}_n\boldsymbol{\mu}_n^\mathsf{T} + \Sigma)\right]\right]$$

The M step for Factor Analysis

M step: Find θ_{t+1} by maximising $\mathcal{F} = \sum_n \langle \log p(\mathbf{z}_n|\theta) + \log p(\mathbf{x}_n|\mathbf{z}_n, \theta) \rangle_{q_n(\mathbf{z}_n)} + c$

$\log p(\mathbf{z}_n|\theta) + \log p(\mathbf{x}_n|\mathbf{z}_n, \theta)$

$$= c - \frac{1}{2}\mathbf{z}_n^\mathsf{T}\mathbf{z}_n - \frac{1}{2}\log|\Psi| - \frac{1}{2}(\mathbf{x}_n - \Lambda\mathbf{z}_n)^\mathsf{T}\Psi^{-1}(\mathbf{x}_n - \Lambda\mathbf{z}_n)$$

$$= c' - \frac{1}{2}\log|\Psi| - \frac{1}{2}\left[\mathbf{x}_n^\mathsf{T}\Psi^{-1}\mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n + \mathbf{z}_n^\mathsf{T}\Lambda^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n\right]$$

$$= c' - \frac{1}{2}\log|\Psi| - \frac{1}{2}\left[\mathbf{x}_n^\mathsf{T}\Psi^{-1}\mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n + \mathrm{Tr}\left[\Lambda^\mathsf{T}\Psi^{-1}\Lambda\mathbf{z}_n\mathbf{z}_n^\mathsf{T}\right]\right]$$

Taking expectations wrt $q_n(\mathbf{z}_n)$:

$$= c' - \frac{1}{2}\log|\Psi| - \frac{1}{2}\left[\mathbf{x}_n^\mathsf{T}\Psi^{-1}\mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T}\Psi^{-1}\Lambda\boldsymbol{\mu}_n + \mathrm{Tr}\left[\Lambda^\mathsf{T}\Psi^{-1}\Lambda(\boldsymbol{\mu}_n\boldsymbol{\mu}_n^\mathsf{T} + \Sigma)\right]\right]$$

Note that we don't need to know everything about $q(\mathbf{z}_n)$, just the moments $\langle\mathbf{z}_n\rangle$ and $\langle\mathbf{z}_n\mathbf{z}_n^\mathsf{T}\rangle$. These are the expected sufficient statistics.

The M step for Factor Analysis (cont.)

$$\mathcal{F} = c' - \frac{N}{2} \log |\Psi| - \frac{1}{2} \sum_n \left[\mathbf{x}_n^{\mathsf{T}} \Psi^{-1} \mathbf{x}_n - 2\mathbf{x}_n^{\mathsf{T}} \Psi^{-1} \Lambda \boldsymbol{\mu}_n + \mathrm{Tr} \left[\Lambda^{\mathsf{T}} \Psi^{-1} \Lambda (\boldsymbol{\mu}_n \boldsymbol{\mu}_n^{\mathsf{T}} + \Sigma) \right] \right]$$

The M step for Factor Analysis (cont.)

$$\mathcal{F} = c' - \frac{N}{2} \log |\Psi| - \frac{1}{2} \sum_n \left[\mathbf{x}_n^\mathsf{T} \Psi^{-1} \mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T} \Psi^{-1} \Lambda \boldsymbol{\mu}_n + \mathrm{Tr} \left[\Lambda^\mathsf{T} \Psi^{-1} \Lambda (\boldsymbol{\mu}_n \boldsymbol{\mu}_n^\mathsf{T} + \Sigma) \right] \right]$$

Taking derivatives wrt Λ and Ψ^{-1}, using $\frac{\partial \mathrm{Tr}[AB]}{\partial B} = A^\mathsf{T}$ and $\frac{\partial \log |A|}{\partial A} = A^{-\mathsf{T}}$:

The M step for Factor Analysis (cont.)

$$\mathcal{F} = c' - \frac{N}{2} \log |\Psi| - \frac{1}{2} \sum_n \left[\mathbf{x}_n^\mathsf{T} \Psi^{-1} \mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T} \Psi^{-1} \Lambda \boldsymbol{\mu}_n + \mathrm{Tr} \left[\Lambda^\mathsf{T} \Psi^{-1} \Lambda (\boldsymbol{\mu}_n \boldsymbol{\mu}_n^\mathsf{T} + \Sigma) \right] \right]$$

Taking derivatives wrt Λ and Ψ^{-1}, using $\frac{\partial \mathrm{Tr}[AB]}{\partial B} = A^\mathsf{T}$ and $\frac{\partial \log |A|}{\partial A} = A^{-\mathsf{T}}$:

$$\frac{\partial \mathcal{F}}{\partial \Lambda} = \Psi^{-1} \sum_n \mathbf{x}_n \boldsymbol{\mu}_n^\mathsf{T} - \Psi^{-1} \Lambda \left(N\Sigma + \sum_n \boldsymbol{\mu}_n \boldsymbol{\mu}_n^\mathsf{T} \right) = 0$$

The M step for Factor Analysis (cont.)

$$\mathcal{F} = c' - \frac{N}{2} \log |\Psi| - \frac{1}{2} \sum_n \left[\mathbf{x}_n^\mathsf{T} \Psi^{-1} \mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T} \Psi^{-1} \Lambda \boldsymbol{\mu}_n + \mathrm{Tr}\left[\Lambda^\mathsf{T} \Psi^{-1} \Lambda (\boldsymbol{\mu}_n \boldsymbol{\mu}_n^\mathsf{T} + \Sigma) \right] \right]$$

Taking derivatives wrt Λ and Ψ^{-1}, using $\frac{\partial \mathrm{Tr}[AB]}{\partial B} = A^\mathsf{T}$ and $\frac{\partial \log |A|}{\partial A} = A^{-\mathsf{T}}$:

$$\frac{\partial \mathcal{F}}{\partial \Lambda} = \Psi^{-1} \sum_n \mathbf{x}_n \boldsymbol{\mu}_n^\mathsf{T} - \Psi^{-1} \Lambda \left(N\Sigma + \sum_n \boldsymbol{\mu}_n \boldsymbol{\mu}_n^\mathsf{T} \right) = 0$$

$$\Rightarrow \widehat{\Lambda} = \left(\sum_n \mathbf{x}_n \boldsymbol{\mu}_n^\mathsf{T} \right) \left(N\Sigma + \sum_n \boldsymbol{\mu}_n \boldsymbol{\mu}_n^\mathsf{T} \right)^{-1}$$

The M step for Factor Analysis (cont.)

$$\mathcal{F} = c' - \frac{N}{2} \log |\Psi| - \frac{1}{2} \sum_n \left[\mathbf{x}_n^\mathsf{T} \Psi^{-1} \mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T} \Psi^{-1} \Lambda \boldsymbol{\mu}_n + \mathrm{Tr} \left[\Lambda^\mathsf{T} \Psi^{-1} \Lambda (\boldsymbol{\mu}_n \boldsymbol{\mu}_n^\mathsf{T} + \Sigma) \right] \right]$$

Taking derivatives wrt Λ and Ψ^{-1}, using $\frac{\partial \mathrm{Tr}[AB]}{\partial B} = A^\mathsf{T}$ and $\frac{\partial \log |A|}{\partial A} = A^{-\mathsf{T}}$:

$$\frac{\partial \mathcal{F}}{\partial \Lambda} = \Psi^{-1} \sum_n \mathbf{x}_n \boldsymbol{\mu}_n^\mathsf{T} - \Psi^{-1} \Lambda \left(N\Sigma + \sum_n \boldsymbol{\mu}_n \boldsymbol{\mu}_n^\mathsf{T} \right) = 0$$

$$\Rightarrow \widehat{\Lambda} = \left(\sum_n \mathbf{x}_n \boldsymbol{\mu}_n^\mathsf{T} \right) \left(N\Sigma + \sum_n \boldsymbol{\mu}_n \boldsymbol{\mu}_n^\mathsf{T} \right)^{-1}$$

$$\frac{\partial \mathcal{F}}{\partial \Psi^{-1}} = \frac{N}{2} \Psi - \frac{1}{2} \sum_n \left[\mathbf{x}_n \mathbf{x}_n^\mathsf{T} - \Lambda \boldsymbol{\mu}_n \mathbf{x}_n^\mathsf{T} - \mathbf{x}_n \boldsymbol{\mu}_n^\mathsf{T} \Lambda^\mathsf{T} + \Lambda (\boldsymbol{\mu}_n \boldsymbol{\mu}_n^\mathsf{T} + \Sigma) \Lambda^\mathsf{T} \right]$$

Note: we should actually only take derivatives w.r.t. Ψ_{dd} since Ψ is diagonal.

The M step for Factor Analysis (cont.)

$$\mathcal{F} = c' - \frac{N}{2}\log|\Psi| - \frac{1}{2}\sum_n \left[\mathbf{x}_n^\mathsf{T}\Psi^{-1}\mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T}\Psi^{-1}\Lambda\boldsymbol{\mu}_n + \mathrm{Tr}\left[\Lambda^\mathsf{T}\Psi^{-1}\Lambda(\boldsymbol{\mu}_n\boldsymbol{\mu}_n^\mathsf{T} + \Sigma)\right]\right]$$

Taking derivatives wrt Λ and Ψ^{-1}, using $\frac{\partial \mathrm{Tr}[AB]}{\partial B} = A^\mathsf{T}$ and $\frac{\partial \log|A|}{\partial A} = A^{-\mathsf{T}}$:

$$\frac{\partial \mathcal{F}}{\partial \Lambda} = \Psi^{-1}\sum_n \mathbf{x}_n\boldsymbol{\mu}_n^\mathsf{T} - \Psi^{-1}\Lambda\left(N\Sigma + \sum_n \boldsymbol{\mu}_n\boldsymbol{\mu}_n^\mathsf{T}\right) = 0$$

$$\Rightarrow \widehat{\Lambda} = \left(\sum_n \mathbf{x}_n\boldsymbol{\mu}_n^\mathsf{T}\right)\left(N\Sigma + \sum_n \boldsymbol{\mu}_n\boldsymbol{\mu}_n^\mathsf{T}\right)^{-1}$$

$$\frac{\partial \mathcal{F}}{\partial \Psi^{-1}} = \frac{N}{2}\Psi - \frac{1}{2}\sum_n \left[\mathbf{x}_n\mathbf{x}_n^\mathsf{T} - \Lambda\boldsymbol{\mu}_n\mathbf{x}_n^\mathsf{T} - \mathbf{x}_n\boldsymbol{\mu}_n^\mathsf{T}\Lambda^\mathsf{T} + \Lambda(\boldsymbol{\mu}_n\boldsymbol{\mu}_n^\mathsf{T} + \Sigma)\Lambda^\mathsf{T}\right]$$

$$\Rightarrow \widehat{\Psi} = \frac{1}{N}\sum_n \left[\mathbf{x}_n\mathbf{x}_n^\mathsf{T} - \Lambda\boldsymbol{\mu}_n\mathbf{x}_n^\mathsf{T} - \mathbf{x}_n\boldsymbol{\mu}_n^\mathsf{T}\Lambda^\mathsf{T} + \Lambda(\boldsymbol{\mu}_n\boldsymbol{\mu}_n^\mathsf{T} + \Sigma)\Lambda^\mathsf{T}\right]$$

Note: we should actually only take derivatives w.r.t. Ψ_{dd} since Ψ is diagonal.

The M step for Factor Analysis (cont.)

$$\mathcal{F} = c' - \frac{N}{2} \log |\Psi| - \frac{1}{2} \sum_n \left[\mathbf{x}_n^\mathsf{T} \Psi^{-1} \mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T} \Psi^{-1} \Lambda \boldsymbol{\mu}_n + \mathrm{Tr} \left[\Lambda^\mathsf{T} \Psi^{-1} \Lambda (\boldsymbol{\mu}_n \boldsymbol{\mu}_n^\mathsf{T} + \Sigma) \right] \right]$$

Taking derivatives wrt Λ and Ψ^{-1}, using $\frac{\partial \mathrm{Tr}[AB]}{\partial B} = A^\mathsf{T}$ and $\frac{\partial \log |A|}{\partial A} = A^{-\mathsf{T}}$:

$$\frac{\partial \mathcal{F}}{\partial \Lambda} = \Psi^{-1} \sum_n \mathbf{x}_n \boldsymbol{\mu}_n^\mathsf{T} - \Psi^{-1} \Lambda \left(N\Sigma + \sum_n \boldsymbol{\mu}_n \boldsymbol{\mu}_n^\mathsf{T} \right) = 0$$

$$\Rightarrow \widehat{\Lambda} = \left(\sum_n \mathbf{x}_n \boldsymbol{\mu}_n^\mathsf{T} \right) \left(N\Sigma + \sum_n \boldsymbol{\mu}_n \boldsymbol{\mu}_n^\mathsf{T} \right)^{-1}$$

$$\frac{\partial \mathcal{F}}{\partial \Psi^{-1}} = \frac{N}{2} \Psi - \frac{1}{2} \sum_n \left[\mathbf{x}_n \mathbf{x}_n^\mathsf{T} - \Lambda \boldsymbol{\mu}_n \mathbf{x}_n^\mathsf{T} - \mathbf{x}_n \boldsymbol{\mu}_n^\mathsf{T} \Lambda^\mathsf{T} + \Lambda (\boldsymbol{\mu}_n \boldsymbol{\mu}_n^\mathsf{T} + \Sigma) \Lambda^\mathsf{T} \right]$$

$$\Rightarrow \widehat{\Psi} = \frac{1}{N} \sum_n \left[\mathbf{x}_n \mathbf{x}_n^\mathsf{T} - \Lambda \boldsymbol{\mu}_n \mathbf{x}_n^\mathsf{T} - \mathbf{x}_n \boldsymbol{\mu}_n^\mathsf{T} \Lambda^\mathsf{T} + \Lambda (\boldsymbol{\mu}_n \boldsymbol{\mu}_n^\mathsf{T} + \Sigma) \Lambda^\mathsf{T} \right]$$

$$\widehat{\Psi} = \Lambda \Sigma \Lambda^\mathsf{T} + \frac{1}{N} \sum_n (\mathbf{x}_n - \Lambda \boldsymbol{\mu}_n)(\mathbf{x}_n - \Lambda \boldsymbol{\mu}_n)^\mathsf{T} \qquad \text{(squared residuals)}$$

Note: we should actually only take derivatives w.r.t. Ψ_{dd} since Ψ is diagonal.

The M step for Factor Analysis (cont.)

$$\mathcal{F} = c' - \frac{N}{2}\log|\Psi| - \frac{1}{2}\sum_n \left[\mathbf{x}_n^\mathsf{T}\Psi^{-1}\mathbf{x}_n - 2\mathbf{x}_n^\mathsf{T}\Psi^{-1}\Lambda\boldsymbol{\mu}_n + \mathrm{Tr}\left[\Lambda^\mathsf{T}\Psi^{-1}\Lambda(\boldsymbol{\mu}_n\boldsymbol{\mu}_n^\mathsf{T} + \Sigma)\right]\right]$$

Taking derivatives wrt Λ and Ψ^{-1}, using $\frac{\partial \mathrm{Tr}[AB]}{\partial B} = A^\mathsf{T}$ and $\frac{\partial \log|A|}{\partial A} = A^{-\mathsf{T}}$:

$$\frac{\partial \mathcal{F}}{\partial \Lambda} = \Psi^{-1}\sum_n \mathbf{x}_n\boldsymbol{\mu}_n^\mathsf{T} - \Psi^{-1}\Lambda\left(N\Sigma + \sum_n \boldsymbol{\mu}_n\boldsymbol{\mu}_n^\mathsf{T}\right) = 0$$

$$\Rightarrow \widehat{\Lambda} = \left(\sum_n \mathbf{x}_n\boldsymbol{\mu}_n^\mathsf{T}\right)\left(N\Sigma + \sum_n \boldsymbol{\mu}_n\boldsymbol{\mu}_n^\mathsf{T}\right)^{-1}$$

$$\frac{\partial \mathcal{F}}{\partial \Psi^{-1}} = \frac{N}{2}\Psi - \frac{1}{2}\sum_n \left[\mathbf{x}_n\mathbf{x}_n^\mathsf{T} - \Lambda\boldsymbol{\mu}_n\mathbf{x}_n^\mathsf{T} - \mathbf{x}_n\boldsymbol{\mu}_n^\mathsf{T}\Lambda^\mathsf{T} + \Lambda(\boldsymbol{\mu}_n\boldsymbol{\mu}_n^\mathsf{T} + \Sigma)\Lambda^\mathsf{T}\right]$$

$$\Rightarrow \widehat{\Psi} = \frac{1}{N}\sum_n \left[\mathbf{x}_n\mathbf{x}_n^\mathsf{T} - \Lambda\boldsymbol{\mu}_n\mathbf{x}_n^\mathsf{T} - \mathbf{x}_n\boldsymbol{\mu}_n^\mathsf{T}\Lambda^\mathsf{T} + \Lambda(\boldsymbol{\mu}_n\boldsymbol{\mu}_n^\mathsf{T} + \Sigma)\Lambda^\mathsf{T}\right]$$

$$\widehat{\Psi} = \Lambda\Sigma\Lambda^\mathsf{T} + \frac{1}{N}\sum_n (\mathbf{x}_n - \Lambda\boldsymbol{\mu}_n)(\mathbf{x}_n - \Lambda\boldsymbol{\mu}_n)^\mathsf{T} \qquad \text{(squared residuals)}$$

Note: we should actually only take derivatives w.r.t. Ψ_{dd} since Ψ is diagonal.
As $\Sigma \to 0$ these become the equations for ML linear regression

Mixtures of Factor Analysers

Simultaneous clustering and dimensionality reduction.

$$p(\mathbf{x}|\theta) = \sum_k \pi_k \, \mathcal{N}(\boldsymbol{\mu}_k, \Lambda_k \Lambda_k^\mathsf{T} + \Psi)$$

where π_k is the mixing proportion for FA k, $\boldsymbol{\mu}_k$ is its centre, Λ_k is its "factor loading matrix", and Ψ is a common sensor noise model. $\theta = \{\{\pi_k, \boldsymbol{\mu}_k, \Lambda_k\}_{k=1\ldots K}, \Psi\}$

We can think of this model as having *two* sets of hidden latent variables:

- A discrete indicator variable $s_n \in \{1, \ldots K\}$
- For each factor analyzer, a continous factor vector $\mathbf{z}_{n,k} \in \mathcal{R}^{D_k}$

$$p(\mathbf{x}|\theta) = \sum_{s_n=1}^{K} p(s_n|\theta) \int p(\mathbf{z}|s_n, \theta) p(\mathbf{x}_n|\mathbf{z}, s_n, \theta) \, d\mathbf{z}$$

As before, an EM algorithm can be derived for this model:

E step: We need moments of $p(\mathbf{z}_n, s_n|\mathbf{x}_n, \theta)$, specifically: $\langle \delta_{s_n=m} \rangle$, $\langle \delta_{s_n=m}\mathbf{z}_n \rangle$ and $\langle \delta_{s_n=m}\mathbf{z}_n\mathbf{z}_n^\mathsf{T} \rangle$.

M step: Similar to M-step for FA with responsibility-weighted moments.
See http://www.learning.eng.cam.ac.uk/zoubin/papers/tr-96-1.pdf

EM for exponential families

EM is often applied to models whose **joint** over $\boldsymbol{\xi} = (\mathbf{z}, \mathbf{x})$ has exponential-family form:

$$p(\boldsymbol{\xi}|\theta) = f(\boldsymbol{\xi}) \exp\{\theta^{\mathsf{T}} \mathsf{T}(\boldsymbol{\xi})\}/Z(\theta)$$

$\left(\text{with } Z(\theta) = \int f(\boldsymbol{\xi}) \exp\{\theta^{\mathsf{T}} \mathsf{T}(\boldsymbol{\xi})\} d\boldsymbol{\xi}\right)$ but whose marginal $p(\mathbf{x}) \notin$ *ExpFam*.

EM for exponential families

EM is often applied to models whose **joint** over $\boldsymbol{\xi} = (\mathbf{z}, \mathbf{x})$ has exponential-family form:

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$\left(\text{with } Z(\theta) = \int f(\boldsymbol{\xi}) \exp\{\theta^{\mathsf{T}}\mathsf{T}(\boldsymbol{\xi})\}d\boldsymbol{\xi}\right)$ but whose marginal $p(\mathbf{x}) \notin \textit{ExpFam}$.
The free energy dependence on θ is given by:

$$\mathcal{F}(q, \theta) = \int q(\mathbf{z}) \log p(\mathbf{z}, \mathbf{x}|\theta)d\mathbf{z} + \mathbf{H}[q]$$

EM for exponential families

EM is often applied to models whose **joint** over $\boldsymbol{\xi} = (\mathbf{z}, \mathbf{x})$ has exponential-family form:

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\end{aligned}$$

So, in the **E step** all we need to compute are the expected sufficient statistics under q.

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The free energy dependence on θ is given by:

$$
\begin{aligned}
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&= \int \underbrace{\tfrac{1}{Z(\theta)} f(\boldsymbol{\xi}) \exp\{\theta^{\mathsf{T}} \mathsf{T}(\boldsymbol{\xi})\}}_{p(\boldsymbol{\xi}|\theta)} \cdot \mathsf{T}(\boldsymbol{\xi}) = \langle \mathsf{T}(\boldsymbol{\xi}) \rangle_{p(\boldsymbol{\xi}|\theta)}
\end{aligned}$$

Thus, the **M step** solves:
$$\frac{\partial \mathcal{F}}{\partial \theta} = \langle \mathsf{T}(\mathbf{z}, \mathbf{x}) \rangle_{q(\mathbf{z})} - \langle \mathsf{T}(\mathbf{z}, \mathbf{x}) \rangle_{p(\boldsymbol{\xi}|\theta)} = 0$$

EM for exponential family mixtures

To derive EM formally for models with discrete latents (including mixtures) it is useful to introduce an indicator vector $\mathbf{s}$ in place of the discrete s.

$$s_i = m \quad \Leftrightarrow \quad \mathbf{s}_i = [0, 0, \ldots, \underbrace{1}_{m\text{th position}}, \ldots 0]$$

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Collecting the M component distributions' natural params into a matrix $\Theta = [\boldsymbol{\theta}_m]$:

$$\log P(\mathcal{X}, \mathcal{S}) = \sum_i \left[(\log \boldsymbol{\pi})^\mathsf{T} \mathbf{s}_i + \mathbf{s}_i^\mathsf{T} \Theta^\mathsf{T} T(\mathbf{x}_i) - \mathbf{s}_i^\mathsf{T} \log \mathbf{Z}(\Theta) \right] + const$$

where $\log \mathbf{Z}(\Theta)$ collects the log-normalisers for all components into an M-element vector.

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$$\sum_i \langle \mathbf{s}_i \rangle_q \qquad \text{(responsibilities } r_{im})$$

$$\sum_i T(\mathbf{x}_i) \left\langle \mathbf{s}_i^\mathsf{T} \right\rangle_q \qquad \text{(responsibility-weighted sufficient stats)}$$

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And maximisation of the expected log-joint (M-step) gives:

$$\boldsymbol{\pi}^{(k+1)} \propto \sum_i \langle \mathbf{s}_i \rangle_q$$

$$\left\langle T(\mathbf{x}) | \boldsymbol{\theta}_m^{(k+1)} \right\rangle = \left(\sum_i T(\mathbf{x}_i) \langle [\mathbf{s}_i]_m \rangle_q \right) \Big/ \left(\sum_i \langle [\mathbf{s}_i]_m \rangle_q \right)$$

EM for MAP

What if we have a prior?

$$p(\boldsymbol{\xi}|\theta) = f(\boldsymbol{\xi})\exp\{\theta^{\mathsf{T}}\mathsf{T}(\boldsymbol{\xi})\}/Z(\theta) \qquad\qquad p(\theta) = F(\nu, \boldsymbol{\tau})\exp\{\theta^{\mathsf{T}}\boldsymbol{\tau}\}/Z(\theta)^{\nu}$$

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Augment the free energy by adding the log prior:

$$\mathcal{F}(q, \theta) = \int q(\mathcal{Z}) \log p(\mathcal{Z}, \mathcal{X}|\theta) d\mathcal{Z} + \mathsf{H}[q] \quad \leq \log P(\mathcal{X}|\theta)$$

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So, the expected sufficient statistics in the E step are unchanged.

Thus, after an E-step the augmented free-energy equals the log-joint, and so free-energy maxima are log-joint maxima (i.e. MAP values).

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Can we find posteriors?

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So, the expected sufficient statistics in the E step are unchanged.

Thus, after an E-step the augmented free-energy equals the log-joint, and so free-energy maxima are log-joint maxima (i.e. MAP values).

Can we find posteriors? Only approximately – we'll return to this later as "Variational Bayes".

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Proof of the Matrix Inversion Lemma

$$(A + XBX^\mathsf{T})^{-1} = A^{-1} - A^{-1}X(B^{-1} + X^\mathsf{T}A^{-1}X)^{-1}X^\mathsf{T}A^{-1}$$

Need to prove:

$$\left(A^{-1} - A^{-1}X(B^{-1} + X^\mathsf{T}A^{-1}X)^{-1}X^\mathsf{T}A^{-1}\right)(A + XBX^\mathsf{T}) = I$$

Expand:

$$I + A^{-1}XBX^\mathsf{T} - A^{-1}X(B^{-1} + X^\mathsf{T}A^{-1}X)^{-1}X^\mathsf{T} - A^{-1}X(B^{-1} + X^\mathsf{T}A^{-1}X)^{-1}X^\mathsf{T}A^{-1}XBX^\mathsf{T}$$

Regroup:

$$= I + A^{-1}X\left(BX^\mathsf{T} - (B^{-1} + X^\mathsf{T}A^{-1}X)^{-1}X^\mathsf{T} - (B^{-1} + X^\mathsf{T}A^{-1}X)^{-1}X^\mathsf{T}A^{-1}XBX^\mathsf{T}\right)$$

$$= I + A^{-1}X\left(BX^\mathsf{T} - (B^{-1} + X^\mathsf{T}A^{-1}X)^{-1}B^{-1}BX^\mathsf{T} - (B^{-1} + X^\mathsf{T}A^{-1}X)^{-1}X^\mathsf{T}A^{-1}XBX^\mathsf{T}\right)$$

$$= I + A^{-1}X\left(BX^\mathsf{T} - (B^{-1} + X^\mathsf{T}A^{-1}X)^{-1}(B^{-1} + X^\mathsf{T}A^{-1}X)BX^\mathsf{T}\right)$$

$$= I + A^{-1}X(BX^\mathsf{T} - BX^\mathsf{T}) = I$$

KL$[q(x)\|p(x)] \geq 0$, **with equality iff** $\forall x : p(x) = q(x)$

First consider discrete distributions; the Kullback-Liebler divergence is:

$$\text{KL}[q\|p] = \sum_i q_i \log \frac{q_i}{p_i}.$$

To minimize wrt distribution q we need a Lagrange multiplier to enforce normalisation:

$$E \overset{\text{def}}{=} \text{KL}[q\|p] + \lambda\left(1 - \sum_i q_i\right) = \sum_i q_i \log \frac{q_i}{p_i} + \lambda\left(1 - \sum_i q_i\right)$$

Find conditions for stationarity

$$\begin{aligned}
\frac{\partial E}{\partial q_i} &= \log q_i - \log p_i + 1 - \lambda = 0 \Rightarrow q_i = p_i \exp(\lambda - 1) \\
\frac{\partial E}{\partial \lambda} &= 1 - \sum_i q_i = 0 \Rightarrow \sum_i q_i = 1
\end{aligned}\right\} \Rightarrow q_i = p_i.$$

Check sign of curvature (Hessian):

$$\frac{\partial^2 E}{\partial q_i \partial q_i} = \frac{1}{q_i} > 0, \qquad \frac{\partial^2 E}{\partial q_i \partial q_j} = 0,$$

so unique stationary point $q_i = p_i$ is indeed a minimum. Easily verified that at that minimum, **KL**$[q\|p] = $ **KL**$[p\|p] = 0$.

A similar proof holds for continuous densities, using functional derivatives.

Fixed Points of EM are Stationary Points in ℓ

Let a fixed point of EM occur with parameter θ^*. Then:

$$\frac{\partial}{\partial \theta} \langle \log P(\mathcal{Z}, \mathcal{X} \mid \theta) \rangle_{P(\mathcal{Z} \mid \mathcal{X}, \theta^*)} \bigg|_{\theta^*} = 0$$

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Now, $\quad \ell(\theta) = \log P(\mathcal{X} \mid \theta) = \langle \log P(\mathcal{X} \mid \theta) \rangle_{P(\mathcal{Z} \mid \mathcal{X}, \theta^*)}$

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$$= \left\langle \log \frac{P(\mathcal{Z}, \mathcal{X}|\theta)}{P(\mathcal{Z}|\mathcal{X}, \theta)} \right\rangle_{P(\mathcal{Z}|\mathcal{X}, \theta^*)}$$

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$$= \langle \log P(\mathcal{Z}, \mathcal{X}|\theta) \rangle_{P(\mathcal{Z}|\mathcal{X}, \theta^*)} - \langle \log P(\mathcal{Z}|\mathcal{X}, \theta) \rangle_{P(\mathcal{Z}|\mathcal{X}, \theta^*)}$$

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Now,

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\ell(\theta) = \log P(\mathcal{X}|\theta) &= \langle \log P(\mathcal{X}|\theta) \rangle_{P(\mathcal{Z}|\mathcal{X}, \theta^*)} \\
&= \left\langle \log \frac{P(\mathcal{Z}, \mathcal{X}|\theta)}{P(\mathcal{Z}|\mathcal{X}, \theta)} \right\rangle_{P(\mathcal{Z}|\mathcal{X}, \theta^*)} \\
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\end{aligned}$$

so,

$$\frac{d}{d\theta} \ell(\theta) = \frac{d}{d\theta} \langle \log P(\mathcal{Z}, \mathcal{X}|\theta) \rangle_{P(\mathcal{Z}|\mathcal{X}, \theta^*)} - \frac{d}{d\theta} \langle \log P(\mathcal{Z}|\mathcal{X}, \theta) \rangle_{P(\mathcal{Z}|\mathcal{X}, \theta^*)}$$

Fixed Points of EM are Stationary Points in ℓ

Let a fixed point of EM occur with parameter θ^*. Then:

$$\frac{\partial}{\partial \theta} \langle \log P(\mathcal{Z}, \mathcal{X} \mid \theta) \rangle_{P(\mathcal{Z}|\mathcal{X}, \theta^*)} \bigg|_{\theta^*} = 0$$

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The second term is 0 at θ^* if the derivative exists (minimum of **KL**$[\cdot\|\cdot]$), and thus:

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So, EM converges to a stationary point of $\ell(\theta)$.

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Let θ^* now be the parameter value at a local maximum of $\mathcal{F}$ (and thus at a fixed point)

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[... as long as the derivatives exist. They sometimes don't (zero-noise ICA)].