Probabilistic & Unsupervised Learning

The EM algorithm

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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
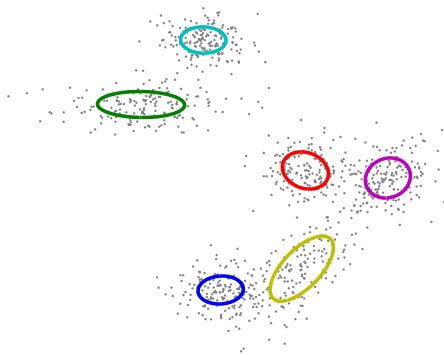
Data: $\mathcal{X} = \{\mathbf{x}_1 \dots \mathbf{x}_N\}$

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

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

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

Log-likelihood:

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

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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. It starts from arbitrary values of the parameters, and iterates two steps:

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▶ How does it work?

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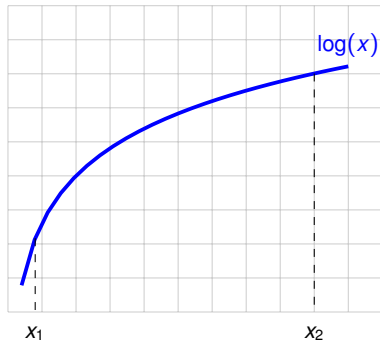
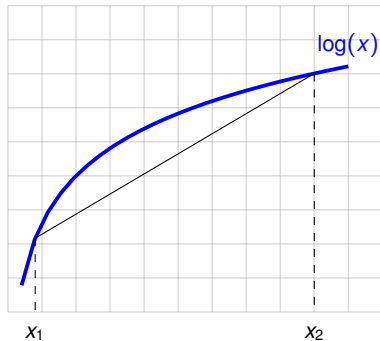# Jensen's inequality

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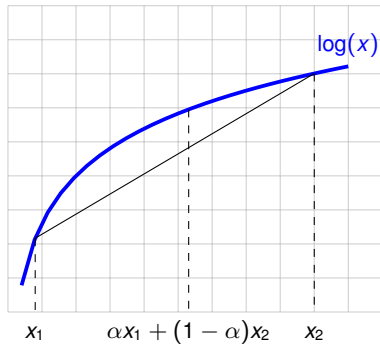One view: EM iteratively refines a lower bound on the log-likelihood.

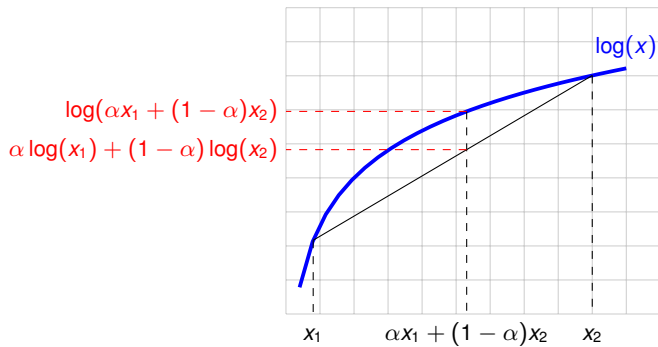# Jensen's inequality

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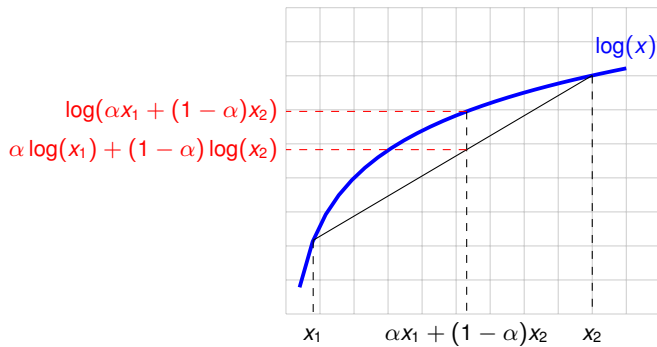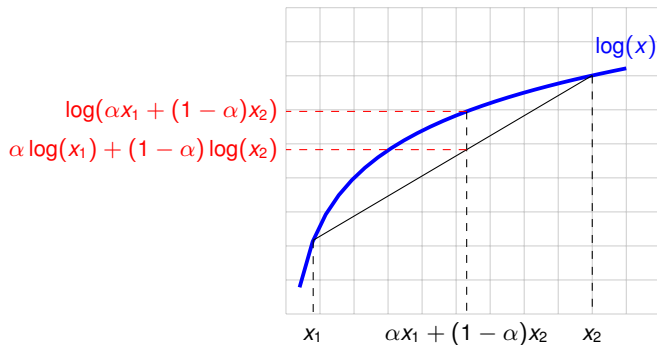
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In general:

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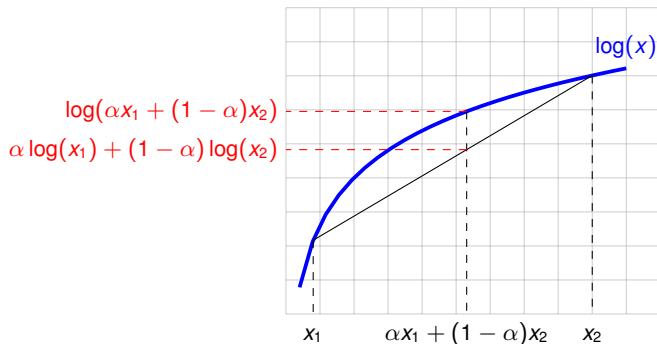One view: EM iteratively refines a lower bound on the log-likelihood.
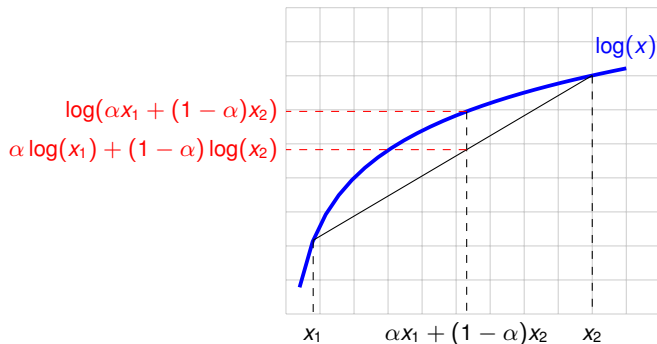
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Equality (if and) only if $f(x)$ is almost surely constant or linear on (convex) support of α.

The lower bound for EM – "free energy"

Observed data $\mathcal{X} = \{\mathbf{x}_i\}$; Latent variables $\mathcal{Y} = \{\mathbf{y}_i\}$; Parameters $\theta = \{\theta_x, \theta_y\}$.

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- **M step:** maximize $\mathcal{F}(q, \theta)$ wrt parameters holding hidden distribution fixed:

$$\theta^{(k)} := \underset{\theta}{\operatorname{argmax}} \ \mathcal{F}\big(q^{(k)}(\mathcal{Y}), \theta\big) = \underset{\theta}{\operatorname{argmax}} \ \langle \log P(\mathcal{Y}, \mathcal{X} | \theta) \rangle_{q^{(k)}(\mathcal{Y})}$$

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

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The free energy can be re-written

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$$\mathcal{F}(q, \theta) = \int q(\mathcal{Y}) \log \frac{P(\mathcal{Y}, \mathcal{X}|\theta)}{q(\mathcal{Y})} \, d\mathcal{Y}$$
$$= \int q(\mathcal{Y}) \log \frac{P(\mathcal{Y}|\mathcal{X}, \theta)P(\mathcal{X}|\theta)}{q(\mathcal{Y})} \, d\mathcal{Y}$$

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$$= \ell(\theta) - \textbf{KL}[q(\mathcal{Y})\|P(\mathcal{Y}|\mathcal{X}, \theta)]$$

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

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

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So, the E step sets

$$q^{(k)}(\mathcal{Y}) = P(\mathcal{Y}|\mathcal{X}, \theta^{(k-1)})$$

and, after an E step, the free energy equals the likelihood.
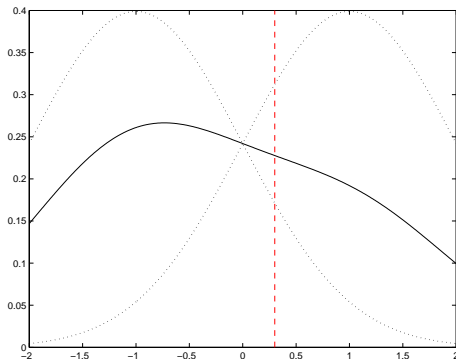
Coordinate Ascent in $\mathcal{F}$ (Demo)

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

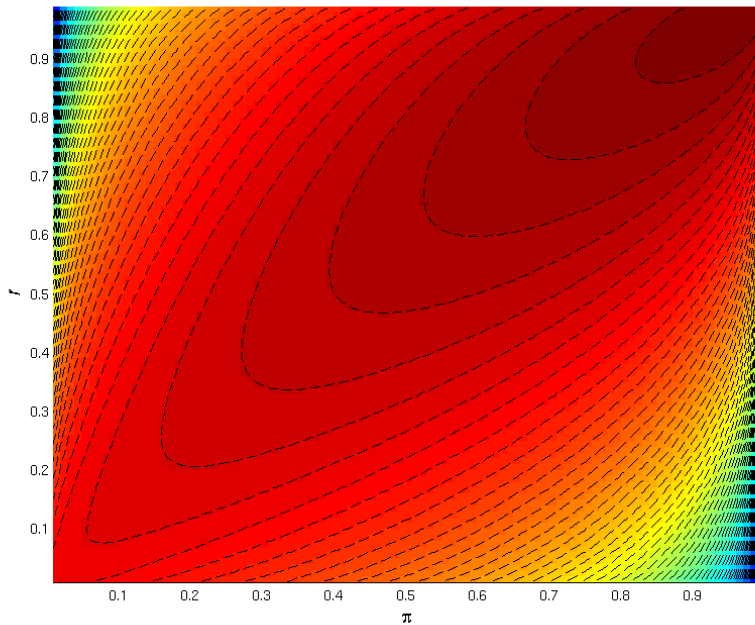$$s \sim \text{Bernoulli}[\pi]$$
$$x|s = 0 \sim \mathcal{N}[-1, 1] \qquad x|s = 1 \sim \mathcal{N}[1, 1].$$

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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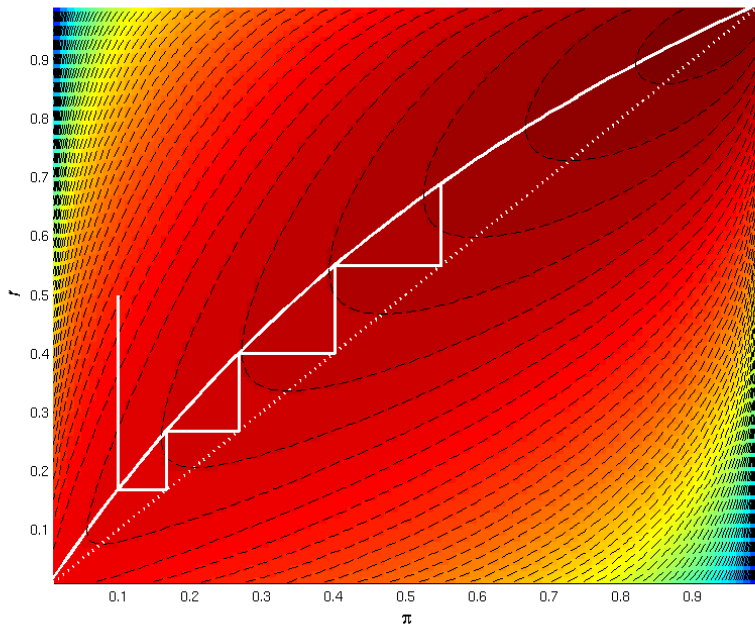
Coordinate Ascent in $\mathcal{F}$ (Demo)
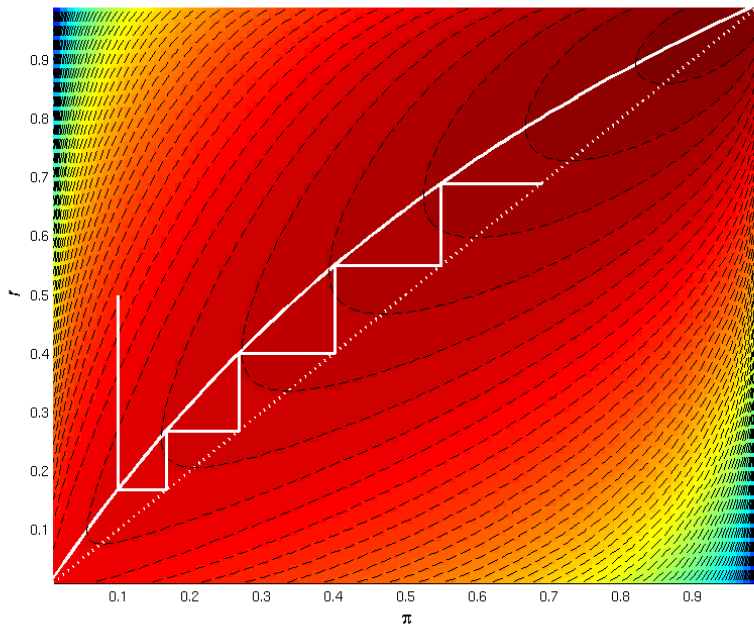
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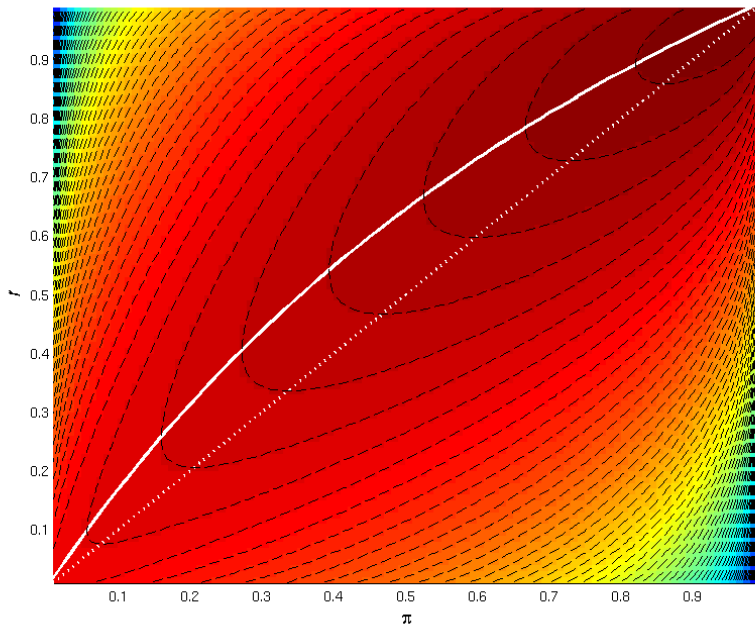# Coordinate Ascent in $\mathcal{F}$ (Demo)
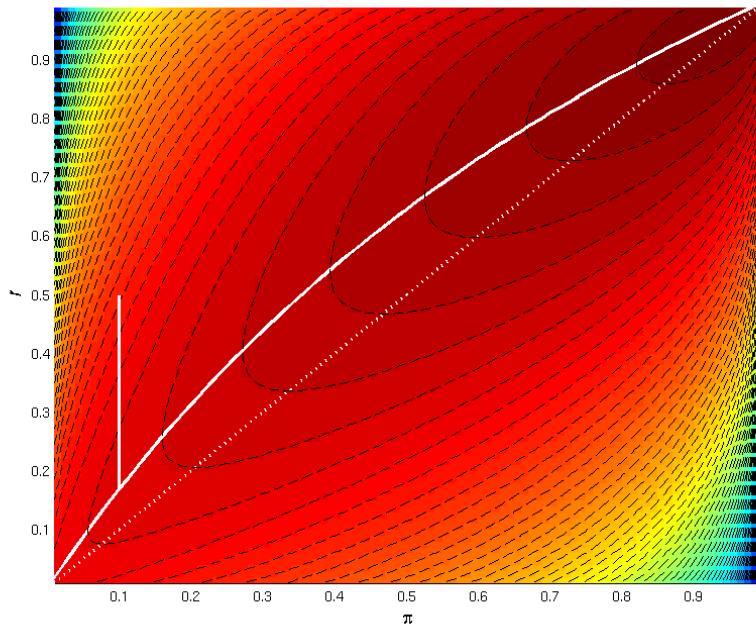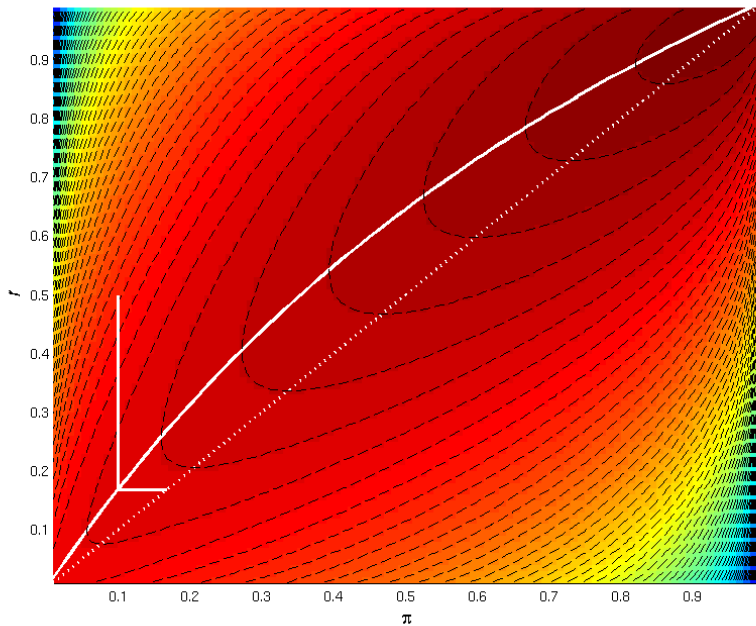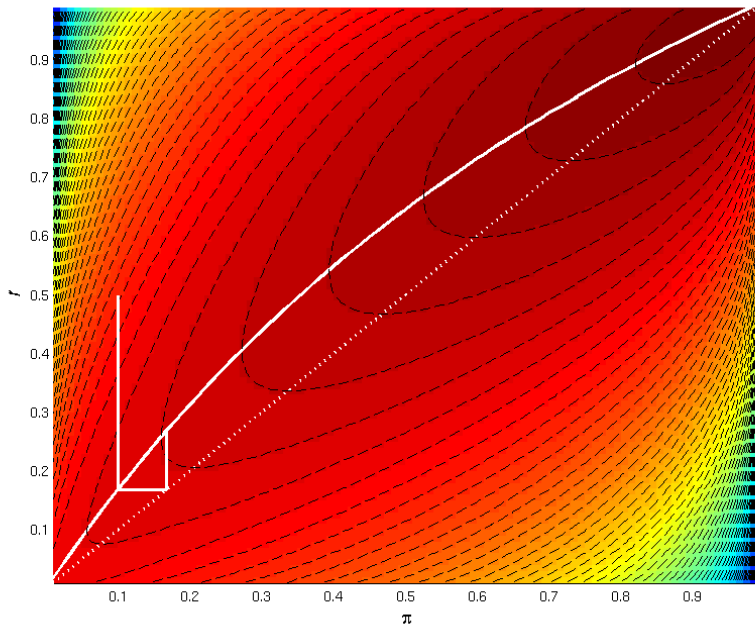
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EM Never Decreases the Likelihood

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

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- The M-step maximises the free energy wrt θ.

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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) correspnd to maxima of the likelihood (see appendices).

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

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

So E-step (inference) can be used to construct other gradient-based optimisation schemes (e.g. "Expectaton 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
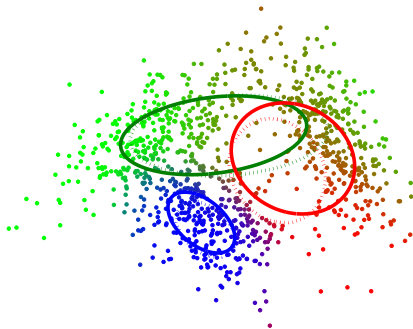
▶ Evaluate responsibilities

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

▶ 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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with the normalization such that $\sum_m r_{im} = 1$.

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

$$E = \langle \log p(x, s|\theta) \rangle_{q(s)} = \sum q(s) \log[p(s|\theta)\, p(x|s, \theta)]$$
$$= \sum_{i,m} r_{im} \Big[\log \pi_m - \log \sigma_m - \frac{1}{2\sigma_m^2}(x_i - \mu_m)^2 \Big].$$

Optimum is found by setting the partial derivatives of E to zero:

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$$
\frac{\partial}{\partial \mu_m} E = \sum_i r_{im} \frac{(x_i - \mu_m)}{2\sigma_m^2} = 0 \;\Rightarrow\; \mu_m = \frac{\sum_i r_{im} x_i}{\sum_i r_{im}},
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$$\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}},$$

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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
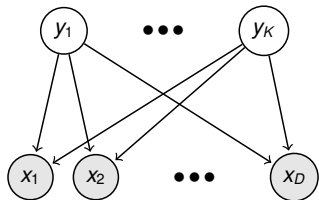
The model for **x**:

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

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: $q_n(\mathbf{y}_n) = p(\mathbf{y}_n|\mathbf{x}_n, \theta_t)$.

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

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

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: $q_n(\mathbf{y}_n) = p(\mathbf{y}_n | \mathbf{x}_n, \theta) = p(\mathbf{y}_n, \mathbf{x}_n | \theta) / p(\mathbf{x}_n | \theta)$

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

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

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 $\mathcal{F} = \sum_n \left\langle \log p(\mathbf{y}_n|\theta) + \log p(\mathbf{x}_n|\mathbf{y}_n, \theta) \right\rangle_{q_n(\mathbf{y}_n)} + c$

The M step for Factor Analysis

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

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

The M step for Factor Analysis

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

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

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

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

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

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

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

The M step for Factor Analysis

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

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

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

The M step for Factor Analysis

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

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

The M step for Factor Analysis

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

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

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

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

The M step for Factor Analysis

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

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

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

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

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

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

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

The M step for Factor Analysis (cont.)

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

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

The M step for Factor Analysis (cont.)

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

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

The M step for Factor Analysis (cont.)

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

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

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 $\frac{\partial \log |A|}{\partial A} = A^{-\mathsf{T}}$:

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

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

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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 $\frac{\partial \log |A|}{\partial A} = A^{-\mathsf{T}}$:

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

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

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

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

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 $\mathbf{y}_{n,k} \in \mathcal{R}^{D_k}$

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

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

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

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 $\mathbf{z} = (\mathbf{y}, \mathbf{x})$ has exponential-family form:

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

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

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The free energy dependence on θ is given by:

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

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The free energy dependence on θ is given by:

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

$$= \int q(\mathbf{y}) \big[\theta^\mathsf{T} \mathsf{T}(\mathbf{z}) - \log Z(\theta)\big] d\mathbf{y} + \text{const wrt } \theta$$

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The free energy dependence on θ is given by:

$$
\begin{aligned}
\mathcal{F}(q, \theta) &= \int q(\mathbf{y}) \log p(\mathbf{y}, \mathbf{x}|\theta) d\mathbf{y} - \mathbf{H}[q] \\
&= \int q(\mathbf{y}) \big[\theta^{\mathsf{T}} \mathsf{T}(\mathbf{z}) - \log Z(\theta)\big] d\mathbf{y} + \text{const wrt } \theta \\
&= \theta^{\mathsf{T}} \langle \mathsf{T}(\mathbf{z}) \rangle_{q(\mathbf{y})} - \log Z(\theta) + \text{const wrt } \theta
\end{aligned}
$$

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

EM for exponential families

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

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

The free energy dependence on θ is given by:

$$
\begin{aligned}
\mathcal{F}(q, \theta) &= \int q(\mathbf{y})\log p(\mathbf{y}, \mathbf{x}|\theta)d\mathbf{y} - \mathbf{H}[q] \\
&= \int q(\mathbf{y})\big[\theta^{\mathsf{T}}\mathsf{T}(\mathbf{z}) - \log Z(\theta)\big]d\mathbf{y} + \text{const wrt } \theta \\
&= \theta^{\mathsf{T}}\langle\mathsf{T}(\mathbf{z})\rangle_{q(\mathbf{y})} - \log Z(\theta) + \text{const wrt } \theta
\end{aligned}
$$

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

$$\frac{\partial}{\partial\theta}\log Z(\theta) = \frac{1}{Z(\theta)}\frac{\partial}{\partial\theta}Z(\theta) = \frac{1}{Z(\theta)}\frac{\partial}{\partial\theta}\int f(\mathbf{z})\exp\{\theta^{\mathsf{T}}\mathsf{T}(\mathbf{z})\}$$

EM for exponential families

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

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

$$\begin{aligned}
\mathcal{F}(q, \theta) &= \int q(\mathbf{y}) \log p(\mathbf{y}, \mathbf{x}|\theta)d\mathbf{y} - \mathbf{H}[q] \\
&= \int q(\mathbf{y})\big[\theta^\mathsf{T}\mathsf{T}(\mathbf{z}) - \log Z(\theta)\big]d\mathbf{y} + \text{const wrt } \theta \\
&= \theta^\mathsf{T}\langle\mathsf{T}(\mathbf{z})\rangle_{q(\mathbf{y})} - \log Z(\theta) + \text{const wrt } \theta
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Thus, the **M step** solves:

$$\frac{\partial \mathcal{F}}{\partial \theta} = \langle \mathsf{T}(\mathbf{z}) \rangle_{q(\mathbf{y})} - \langle \mathsf{T}(\mathbf{z})|\theta \rangle = 0$$

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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:

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

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

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

Find conditions for stationarity

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

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:

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

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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 $\ell(\theta)$.

Maxima in $\mathcal{F}$ correspond to maxima in ℓ

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

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The first term on the right is negative (a maximum) and the second term is positive (a minimum).

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