Unsupervised Learning

The EM Algorithm

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The Expectation Maximization (EM) algorithm

Assume a model with observed (visible) variables $\mathbf{y}$, unobserved (hidden / latent / missing) variables $\mathbf{x}$, and model parameters θ

Goal: Maximize the log likelihood (i.e. ML learning) wrt θ:

$$\mathcal{L}(\theta) = \log p(\mathbf{y}|\theta) = \log \int p(\mathbf{x}, \mathbf{y}|\theta) d\mathbf{x},$$

Any distribution, $q(\mathbf{x})$, over the hidden variables can be used to obtain a lower bound on the log likelihood:

$$\mathcal{L}(\theta) = \log \int q(\mathbf{x}) \frac{p(\mathbf{x}, \mathbf{y}|\theta)}{q(\mathbf{x})} d\mathbf{x} \geq \int q(\mathbf{x}) \log \frac{p(\mathbf{x}, \mathbf{y}|\theta)}{q(\mathbf{x})} \, d\mathbf{x} \overset{\text{def}}{=} \mathcal{F}(q, \theta),$$

This lower bound is called Jensen's inequality and comes from the fact that the log function is concave ("log of average is greater than average of logs").

In the EM algorithm, we alternately optimize $\mathcal{F}(q, \theta)$ wrt $q(\mathbf{x})$ and θ, and we can prove that this will never decrease $\mathcal{L}(\theta)$.

The E and M steps of EM

The lower bound on the log likelihood:

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

where $\mathcal{H}(q) = -\int q(\mathbf{x}) \log q(\mathbf{x}) d\mathbf{x}$ is the entropy of $q(\mathbf{x})$. EM alternates between:

E step: optimize $\mathcal{F}(q,\theta)$ wrt distribution over hidden variables holding parameters fixed:

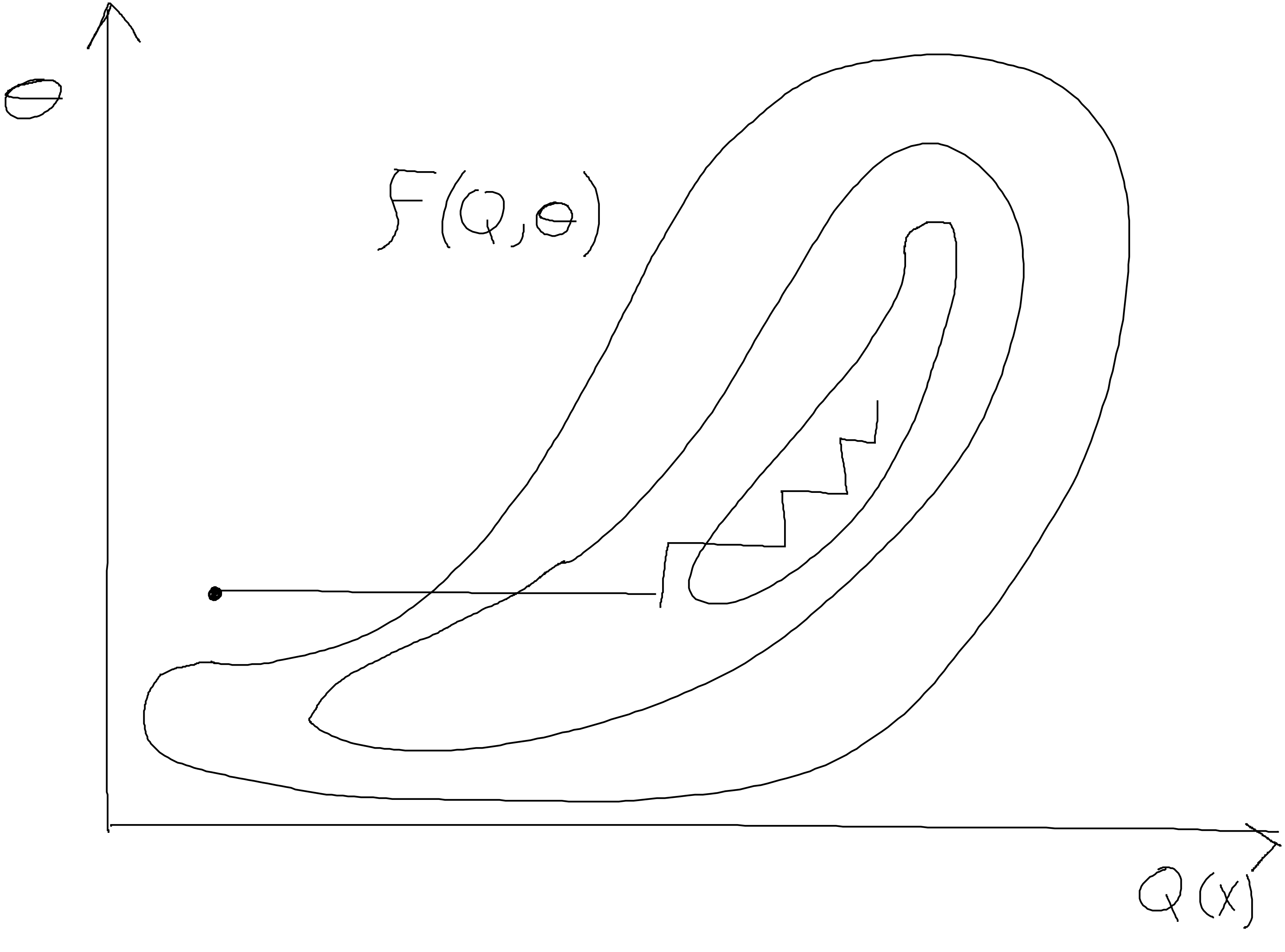
$$q^{(k)}(\mathbf{x}) := \underset{q(\mathbf{x})}{\operatorname{argmax}} \ \mathcal{F}\big(q(\mathbf{x}), \theta^{(k-1)}\big).$$

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

$$\theta^{(k)} := \underset{\theta}{\operatorname{argmax}} \ \mathcal{F}\big(q^{(k)}(\mathbf{x}), \theta\big) = \underset{\theta}{\operatorname{argmax}} \int q^{(k)}(\mathbf{x}) \log p(\mathbf{x},\mathbf{y}|\theta) d\mathbf{x}.$$

The second equality comes from the fact that the entropy of $q(\mathbf{x})$ does not depend directly on θ.

EM as Coordinate Ascent in $\mathcal{F}$



The Intuition Behind EM

E step: fill in values for the hidden variables according to their posterior probabilities

M step: learn model as if hidden variables were not hidden

- EM is useful because in many models, if the hidden variables were no longer hidden, learning would be easy (e.g. consider a mixture of Gaussians).
- EM breaks up a hard learning problem into a sequence of easy learning problems.

The EM algorithm never decreases the log likelihood

The difference between the log likelihood and the lower bound:

$$\begin{aligned}
\mathcal{L}(\theta) - \mathcal{F}(q,\theta) &= \log p(\mathbf{y}|\theta) - \int q(\mathbf{x}) \log \frac{p(\mathbf{x},\mathbf{y}|\theta)}{q(\mathbf{x})} d\mathbf{x} \\
&= \log p(\mathbf{y}|\theta) - \int q(\mathbf{x}) \log \frac{p(\mathbf{x}|\mathbf{y},\theta)p(\mathbf{y}|\theta)}{q(\mathbf{x})} d\mathbf{x} \\
&= -\int q(\mathbf{x}) \log \frac{p(\mathbf{x}|\mathbf{y},\theta)}{q(\mathbf{x})} d\mathbf{x} \ = \ \mathcal{KL}\big(q(\mathbf{x}), p(\mathbf{x}|\mathbf{y},\theta)\big),
\end{aligned}$$

This is the Kullback-Liebler divergence; it is zero if and only if $q(\mathbf{x}) = p(\mathbf{x}|\mathbf{y},\theta)$.

Therefore, the E step simply sets $q(\mathbf{x}) \leftarrow p(\mathbf{x}|\mathbf{y},\theta)$.

The E and M steps together increase the log likelihood:

$$\mathcal{L}\big(\theta^{(k-1)}\big) \underset{\text{E step}}{=} \mathcal{F}\big(q^{(k)}, \theta^{(k-1)}\big) \underset{\text{M step}}{\leq} \mathcal{F}\big(q^{(k)}, \theta^{(k)}\big) \underset{\text{Jensen}}{\leq} \mathcal{L}\big(\theta^{(k)}\big),$$

where the first equality holds because of the E step, and the first inequality comes from the M step and the final inequality from Jensen.

EM converges to a local optimum of $\mathcal{L}(\theta)$.

The $\mathcal{KL}\big(q(x), p(x)\big)$ is non-negative and zero iff $\forall x: \; p(x) = q(x)$

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

$$\mathcal{KL}(q,p) = \sum_i q_i \log \frac{q_i}{p_i}.$$

To find the distribution q which minimizes $\mathcal{KL}(q,p)$ we add a Lagrange multiplier to enforce the normalization constraint:

$$E \overset{\text{def}}{=} \mathcal{KL}(q,p) + \lambda\big(1 - \sum_i q_i\big) = \sum_i q_i \log \frac{q_i}{p_i} + \lambda\big(1 - \sum_i q_i\big)$$

We then take partial derivatives and set to zero:

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

Why $\mathcal{KL}(q,p)$ is non-negative and zero iff $p(x) = q(x)$ . . .

Check that the curvature (Hessian) is positive (definite), corresponding to a minimum:

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

showing that $q_i = p_i$ is a genuine minimum.

At the minimum is it easily verified that $\mathcal{KL}(p,p) = 0$.

A similar proof holds for $\mathcal{KL}$ between continuous densities, the derivatives being substituted by functional derivatives.

The Gaussian mixture model (E-step)

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

$$p(y|\theta) = \sum_{k=1}^{K} p(s=k|\theta)p(y|s=k,\theta) \propto \sum_{k=1}^{K} \frac{\pi_k}{\sigma_k} \exp\big\{-\frac{1}{2\sigma_k^2}(y-\mu_k)^2\big\},$$

where θ is the collection of parameters: means μ_k, variances σ_k^2 and mixing proportions $\pi_k = p(s=k|\theta)$.

The hidden variable $s^{(c)}$ indicates which component observation $y^{(c)}$ belongs to.
The E-step computes the posterior for $s^{(c)}$ given the current parameters:

$$\begin{aligned} q(s^{(c)}) &= p(s^{(c)}|y^{(c)},\theta) \propto p(y^{(c)}|s^{(c)},\theta)p(s^{(c)}|\theta) \\ r_k^{(c)} \overset{\text{def}}{=} q(s^{(c)}=k) &\propto \frac{\pi_k}{\sigma_k} \exp\big\{-\frac{1}{2\sigma_k^2}(y^{(c)}-\mu_k)^2\big\} \qquad \text{(responsibilities)} \end{aligned}$$

with the normalization such that $\sum_k r_k^{(c)} = 1$.

The Gaussian mixture model (M-step)

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

$$E \;=\; \sum q(s)\log[p(s|\theta)\;p(y|s,\theta)] \;=\; \sum_{c,k} r_k^{(c)}\Big[\log\pi_k - \log\sigma_k - \frac{1}{2\sigma_k^2}(y^{(c)}-\mu_k)^2\Big].$$

Optimization is done by setting the partial derivatives of E to zero:

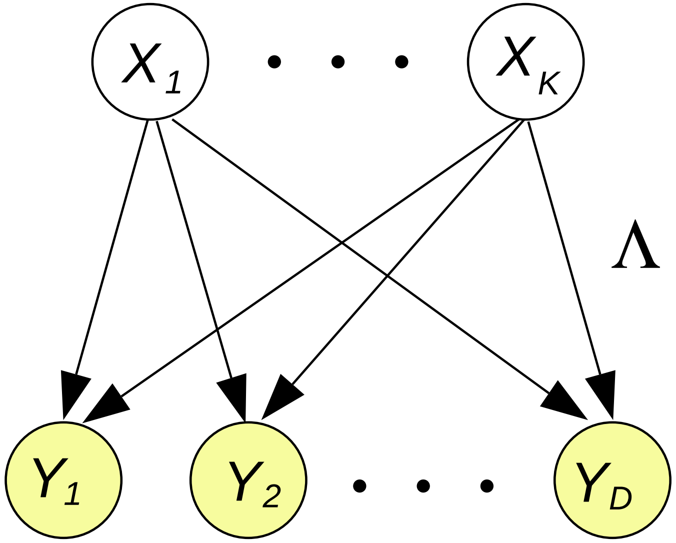
$$\frac{\partial E}{\partial \mu_k} \;=\sum_c r_k^{(c)}\frac{(y^{(c)}-\mu_k)}{2\sigma_k^2} = 0 \Rightarrow \quad \mu_k = \frac{\sum_c r_k^{(c)} y^{(c)}}{\sum_c r_k^{(c)}},$$

$$\frac{\partial E}{\partial \sigma_k} \;=\sum_c r_k^{(c)}\Big[-\frac{1}{\sigma_k}+\frac{(y^{(c)}-\mu_k)^2}{\sigma_k^3}\Big] = 0 \Rightarrow \quad \sigma_k^2 = \frac{\sum_c r_k^{(c)}(y^{(c)}-\mu_k)^2}{\sum_c r_k^{(c)}},$$

$$\frac{\partial E}{\partial \pi_k} \;=\sum_c r_k^{(c)}\frac{1}{\pi_k}, \qquad \frac{\partial E}{\partial \pi_k}+\lambda = 0 \Rightarrow \quad \pi_k = \frac{1}{n}\sum_c r_k^{(c)},$$

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

Factor Analysis



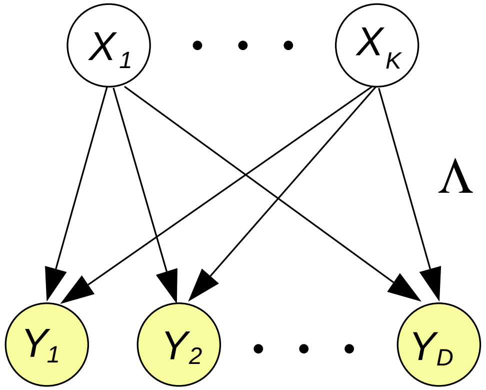
Linear generative model: $y_d = \sum_{k=1}^{K} \Lambda_{dk}\, x_k + \epsilon_d$

- x_k are independent $\mathcal{N}(0,1)$ Gaussian factors
- ϵ_d are independent $\mathcal{N}(0,\Psi_{dd})$ Gaussian noise
- $K < D$

So, $\mathbf{y}$ is Gaussian with: $p(\mathbf{y}) = \int p(\mathbf{x}) p(\mathbf{y}|\mathbf{x}) d\mathbf{x} = \mathcal{N}(0, \Lambda\Lambda^\top + \Psi)$
where Λ is a $D \times K$ matrix, and Ψ is diagonal.

Dimensionality Reduction: Finds a low-dimensional projection of high dimensional data that captures the correlation structure of the data.

EM for Factor Analysis



The model for $\mathbf{y}$:
$p(\mathbf{y}|\theta) = \int p(\mathbf{x}|\theta)p(\mathbf{y}|\mathbf{x},\theta)d\mathbf{x} = \mathcal{N}(0, \Lambda\Lambda^\top + \Psi)$
Model parameters: $\theta = \{\Lambda, \Psi\}$.

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

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

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

The E step for Factor Analysis

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

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

$$\begin{aligned}
p(\mathbf{x}, \mathbf{y}_n) &= p(\mathbf{x})p(\mathbf{y}_n|\mathbf{x}) \\
&= (2\pi)^{-\frac{K}{2}} \exp\{-\frac{1}{2}\mathbf{x}^\top\mathbf{x}\} \; |2\pi\Psi|^{-\frac{1}{2}} \exp\{-\frac{1}{2}(\mathbf{y}_n - \Lambda\mathbf{x})^\top\Psi^{-1}(\mathbf{y}_n - \Lambda\mathbf{x})\} \\
&= \text{c} \times \exp\{-\frac{1}{2}[\mathbf{x}^\top\mathbf{x} + (\mathbf{y}_n - \Lambda\mathbf{x})^\top\Psi^{-1}(\mathbf{y}_n - \Lambda\mathbf{x})]\} \\
&= \text{c'} \times \exp\{-\frac{1}{2}[\mathbf{x}^\top(I + \Lambda^\top\Psi^{-1}\Lambda)\mathbf{x} - 2\mathbf{x}^\top\Lambda^\top\Psi^{-1}\mathbf{y}_n]\} \\
&= \text{c''} \times \exp\{-\frac{1}{2}[\mathbf{x}^\top\Sigma^{-1}\mathbf{x} - 2\mathbf{x}^\top\Sigma^{-1}\mu + \mu^\top\Sigma^{-1}\mu]\}
\end{aligned}$$

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

The M step for Factor Analysis

M step: Find θ_{t+1} maximising $\mathcal{F} = \sum_n \int q_n(\mathbf{x}) \left[\log p(\mathbf{x}|\theta) + \log p(\mathbf{y}_n|\mathbf{x},\theta)\right] d\mathbf{x} + \mathsf{c}$

$$\begin{aligned}
\log p(\mathbf{x}|\theta) + \log p(\mathbf{y}_n|\mathbf{x},\theta) &= \mathsf{c} - \frac{1}{2}\mathbf{x}^\top\mathbf{x} - \frac{1}{2}\log|\Psi| - \frac{1}{2}(\mathbf{y}_n - \Lambda\mathbf{x})^\top\Psi^{-1}(\mathbf{y}_n - \Lambda\mathbf{x}) \\
&= \mathsf{c'} - \frac{1}{2}\log|\Psi| - \frac{1}{2}[\mathbf{y}_n{}^\top\Psi^{-1}\mathbf{y}_n - 2\mathbf{y}_n{}^\top\Psi^{-1}\Lambda\mathbf{x} + \mathbf{x}^\top\Lambda^\top\Psi^{-1}\Lambda\mathbf{x}] \\
&= \mathsf{c'} - \frac{1}{2}\log|\Psi| - \frac{1}{2}[\mathbf{y}_n{}^\top\Psi^{-1}\mathbf{y}_n - 2\mathbf{y}_n{}^\top\Psi^{-1}\Lambda\mathbf{x} + \mathsf{tr}(\Lambda^\top\Psi^{-1}\Lambda\mathbf{x}\mathbf{x}^\top)]
\end{aligned}$$

Taking expectations over $q_n(\mathbf{x})$...

$$= \mathsf{c'} - \frac{1}{2}\log|\Psi| - \frac{1}{2}[\mathbf{y}_n{}^\top\Psi^{-1}\mathbf{y}_n - 2\mathbf{y}_n{}^\top\Psi^{-1}\Lambda\mu_n + \mathsf{tr}(\Lambda^\top\Psi^{-1}\Lambda(\mu_n\mu_n{}^\top + \Sigma))]$$

Note that we don't need to know everything about q, just the expectations of $\mathbf{x}$ and $\mathbf{x}\mathbf{x}^\top$ under q (i.e. the expected sufficient statistics).

The M step for Factor Analysis (cont.)

$$\mathcal{F} = \text{c'} - \frac{N}{2}\log|\Psi| - \frac{1}{2}\sum_n \left[\mathbf{y}_n{}^\top \Psi^{-1}\mathbf{y}_n - 2\mathbf{y}_n{}^\top \Psi^{-1}\Lambda\mu_n + \text{tr}(\Lambda^\top\Psi^{-1}\Lambda(\mu_n\mu_n{}^\top + \Sigma))\right]$$

Taking derivatives w.r.t. Λ and Ψ^{-1}, using $\frac{\partial \text{tr}(AB)}{\partial B} = A^\top$ and $\frac{\partial \log|A|}{\partial A} = A^{-\top}$:

$$\frac{\partial\mathcal{F}}{\partial\Lambda} = \Psi^{-1}\sum_n \mathbf{y}_n\mu_n{}^\top - \Psi^{-1}\Lambda\left(N\Sigma + \sum_n \mu_n\mu_n{}^\top\right) = 0$$

$$\hat{\Lambda} = (\sum_n \mathbf{y}_n\mu_n{}^\top)\left(N\Sigma + \sum_n \mu_n\mu_n{}^\top\right)^{-1}$$

$$\frac{\partial\mathcal{F}}{\partial\Psi^{-1}} = \frac{N}{2}\Psi - \frac{1}{2}\sum_n \left[\mathbf{y}_n\mathbf{y}_n{}^\top - \Lambda\mu_n\mathbf{y}_n{}^\top - \mathbf{y}_n\mu_n{}^\top\Lambda^\top + \Lambda(\mu_n\mu_n{}^\top + \Sigma)\Lambda^\top\right]$$

$$\hat{\Psi} = \frac{1}{N}\sum_n \left[\mathbf{y}_n\mathbf{y}_n{}^\top - \Lambda\mu_n\mathbf{y}_n{}^\top - \mathbf{y}_n\mu_n{}^\top\Lambda^\top + \Lambda(\mu_n\mu_n{}^\top + \Sigma)\Lambda^\top\right]$$

$$\hat{\Psi} = \Lambda\Sigma\Lambda^\top + \frac{1}{N}\sum_n (\mathbf{y}_n - \Lambda\mu_n)(\mathbf{y}_n - \Lambda\mu_n)^\top \qquad \text{(squared residuals)}$$

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

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).

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. You can also update the posterior over a subset of the hidden variables, while holding others fixed...

EM for exponential families

Defn: p is in the exponential family for $\mathbf{z} = (\mathbf{x}, \mathbf{y})$ if it can be written:

$$p(\mathbf{z}|\theta) = b(\mathbf{z}) \exp\{\theta^\top s(\mathbf{z})\}/\alpha(\theta)$$

where $\alpha(\theta) = \int b(\mathbf{z}) \exp\{\theta^\top s(\mathbf{z})\} d\mathbf{z}$

E step: $q(\mathbf{x}) = p(\mathbf{x}|\mathbf{y}, \theta)$

M step: $\theta^{(k)} := \underset{\theta}{\operatorname{argmax}} \; \mathcal{F}(q, \theta)$

$$\begin{aligned} \mathcal{F}(q, \theta) &= \int q(\mathbf{x}) \log p(\mathbf{x}, \mathbf{y}|\theta) d\mathbf{x} - \mathcal{H}(q) \\ &= \int q(\mathbf{x}) [\theta^\top s(\mathbf{z}) - \log \alpha(\theta)] d\mathbf{x} + \text{const} \end{aligned}$$

It is easy to verify that: $\dfrac{\partial \log \alpha(\theta)}{\partial \theta} = E[s(\mathbf{z})|\theta]$

Therefore, M step solves: $\dfrac{\partial \mathcal{F}}{\partial \theta} = E_{q(\mathbf{x})}[s(\mathbf{z})] - E[s(\mathbf{z})|\theta] = 0$

Mixtures of Factor Analysers

Simultaneous clustering and dimensionality reduction.

$$p(\mathbf{y}|\theta) = \sum_k \pi_k \, \mathcal{N}(\mu_k, \Lambda_k \Lambda^\top{}_k + \Psi)$$

where π_k is the mixing proportion for FA k, μ_k is its centre, Λ_k is its "factor loading matrix", and Ψ is a common sensor noise model. $\theta = \{\{\pi_k, \mu_k, \Lambda_k\}_{k=1\ldots K}, \Psi\}$
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 $\mathbf{x}_{n,k} \in \mathcal{R}^{D_k}$

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

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

E step: Infer joint distribution of latent variables, $p(\mathbf{x}_n, s_n|\mathbf{y}_n, \theta)$

M step: Maximize $\mathcal{F}$ with respect to θ.

Proof of the Matrix Inversion Lemma

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

Need to prove:

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

Expand:

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

Regroup:

$$\begin{aligned}
&= \quad I + A^{-1}X\left(BX^\top - (B^{-1} + X^\top A^{-1}X)^{-1}X^\top - (B^{-1} + X^\top A^{-1}X)^{-1}X^\top A^{-1}XBX^\top\right) \\
&= \quad I + A^{-1}X\left(BX^\top - (B^{-1} + X^\top A^{-1}X)^{-1}B^{-1}BX^\top - (B^{-1} + X^\top A^{-1}X)^{-1}X^\top A^{-1}XBX^\top\right) \\
&= \quad I + A^{-1}X\left(BX^\top - (B^{-1} + X^\top A^{-1}X)^{-1}(B^{-1} + X^\top A^{-1}X)BX^\top\right) \\
&= \quad I + A^{-1}X(BX^\top - BX^\top) = I
\end{aligned}$$

Further Readings

- David MacKay's Textbook, Chapters 20, 22 and 23
  http://www.inference.phy.cam.ac.uk/mackay/itprnn/

- Ghahramani, Z. and Hinton, G.E. (1996) The EM Algorithm for Mixtures of Factor Analyzers. University of Toronto Technical Report CRG-TR-96-1
  http://www.gatsby.ucl.ac.uk/∼zoubin/papers/tr-96-1.ps.gz

- Minka, T. Tutorial on linear algebra.
  http://www.stat.cmu.edu/∼minka/papers/matrix.html

- Roweis, S.T. and Ghahramani, Z. (1999) A Unifying Review of Linear Gaussian Models. Neural Computation 11(2). Sections 1-5.3 and 6-6.1. See also Appendix A.1-A.2.
  http://www.gatsby.ucl.ac.uk/∼zoubin/abstracts/lds.abs.html

- Welling, M. (2000) Linear models. class notes.
  http://www.gatsby.ucl.ac.uk/∼zoubin/course03/PCA.ps or /PCA.pdf