

Probabilistic & Unsupervised Learning

Expectation Maximisation

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Log-likelihoods

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

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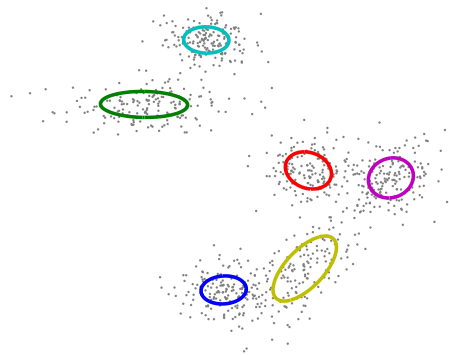
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- ▶ Often multiple local maxima.
- ▶ Direct numerical optimisation may be possible but infrequently easy.

Example: mixture of Gaussians



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

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

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:

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

The joint-data likelihood and EM

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- ▶ **Idea:** update θ and (the distribution on) \mathbf{y} in alternation, to reach a self-consistent answer. **Will this yield the right answer?**
- ▶ 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.

Start from arbitrary values of the parameters, and iterate two steps:

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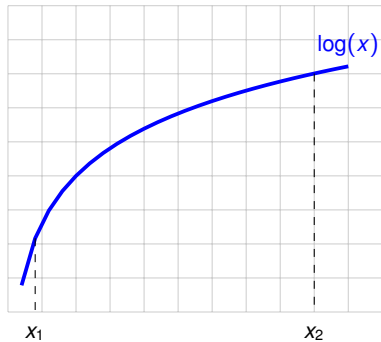
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- ▶ Provides a framework for **principled approximations**.

Jensen's inequality

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

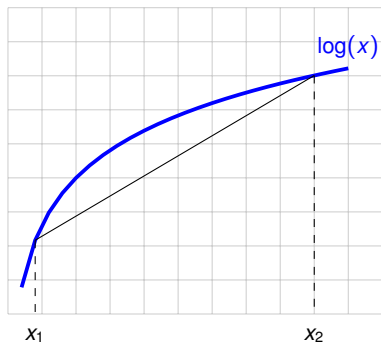
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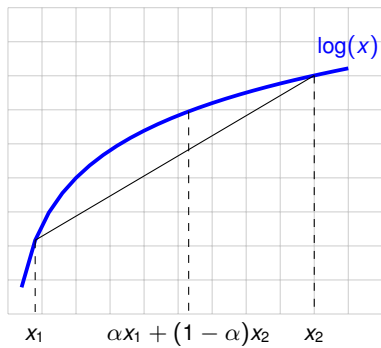
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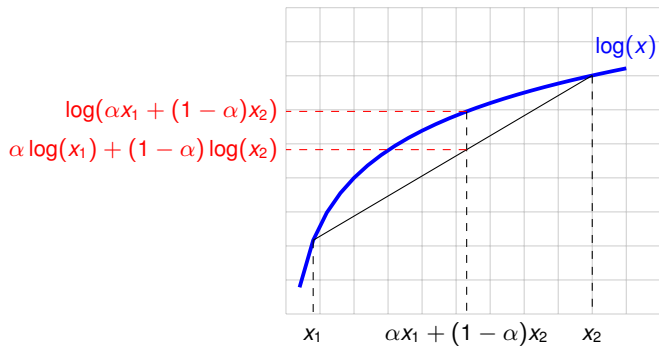
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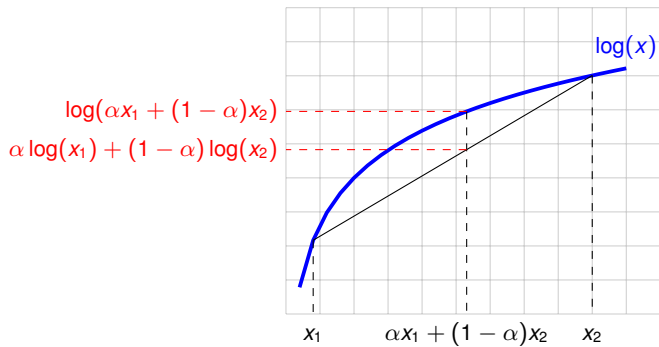
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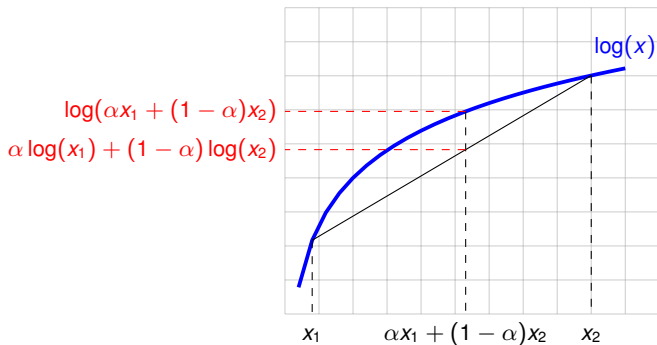
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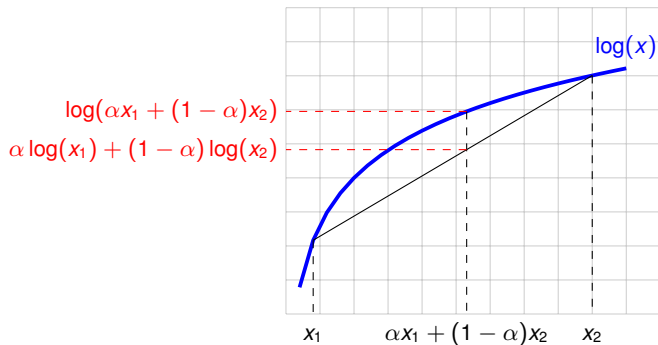
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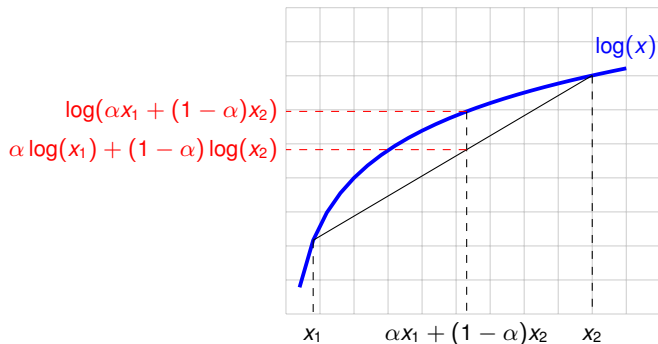
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Equality (if and) only if $f(x)$ is almost surely constant or linear on (convex) support of α .

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

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So:

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

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

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So, the E step sets

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

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

Coordinate Ascent in \mathcal{F} (Demo)

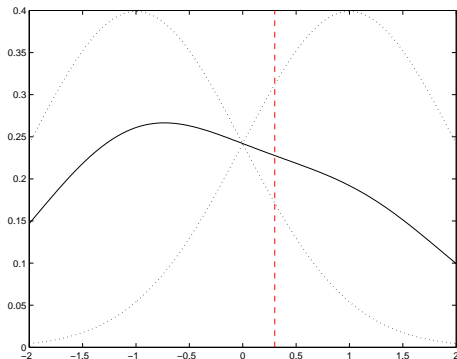
To visualise, we consider a one parameter / one latent mixture:

$$s \sim \text{Bernoulli}[\pi]$$

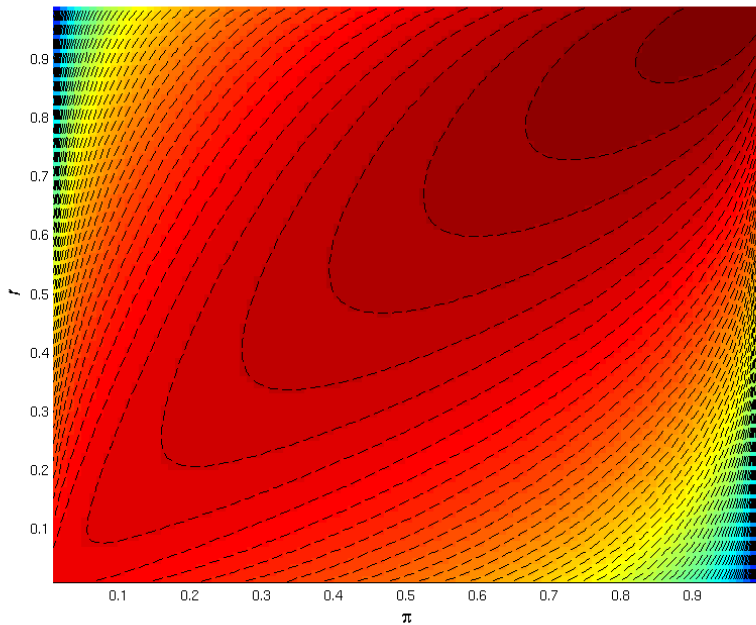
$$x|s = 0 \sim \mathcal{N}[-1, 1] \quad x|s = 1 \sim \mathcal{N}[1, 1].$$

Single data point $x_1 = .3$.

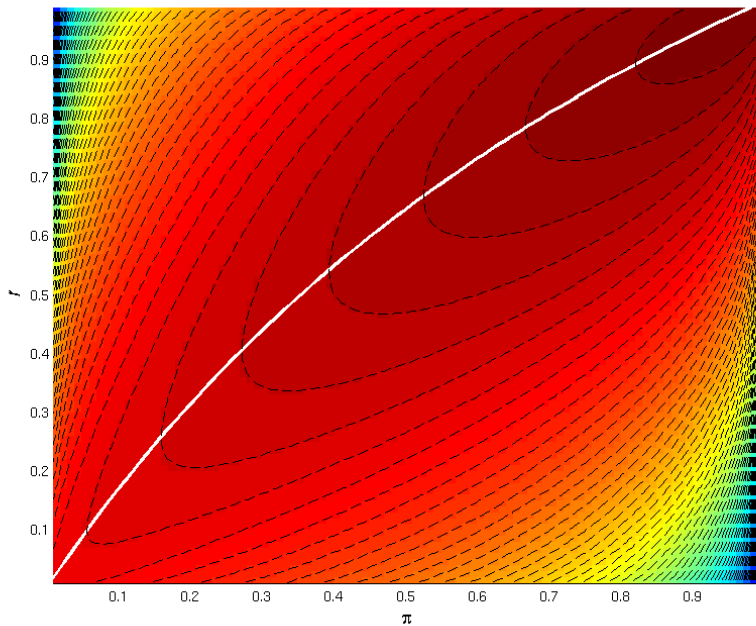
$q(s)$ is a distribution on a single binary latent, and so is represented by $r_1 \in [0, 1]$.



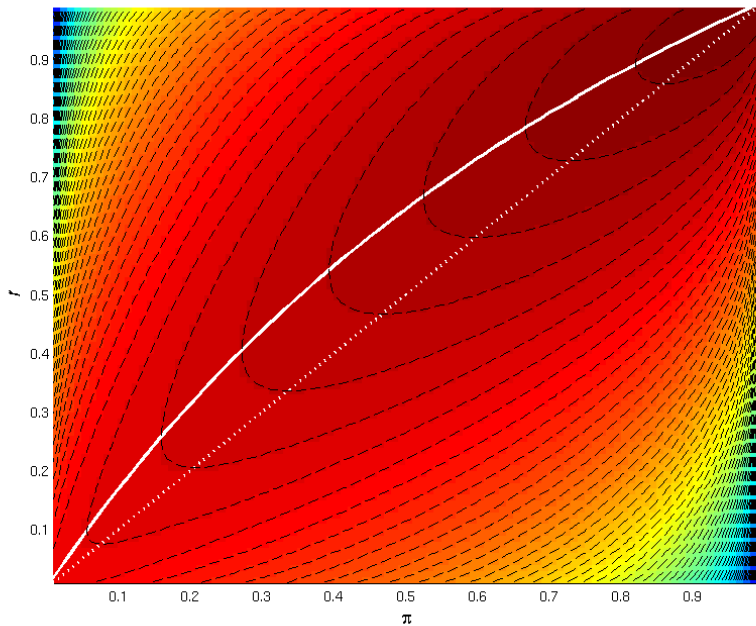
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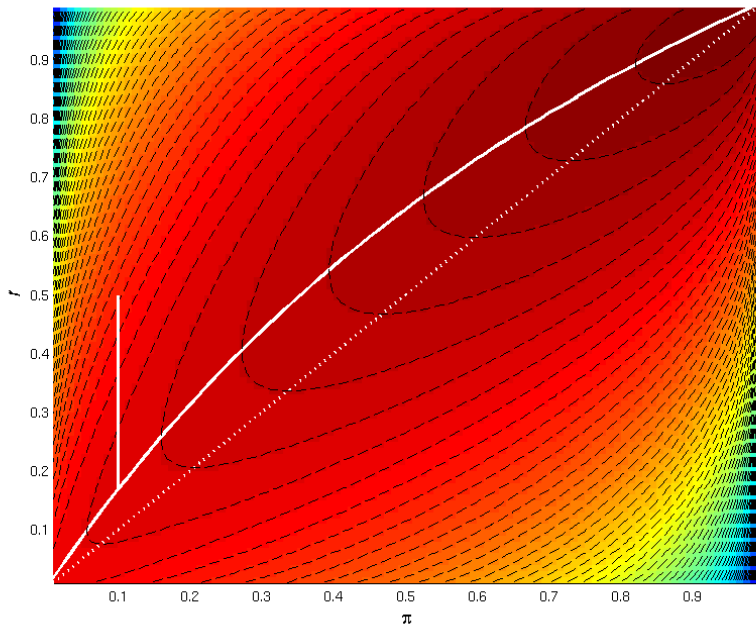
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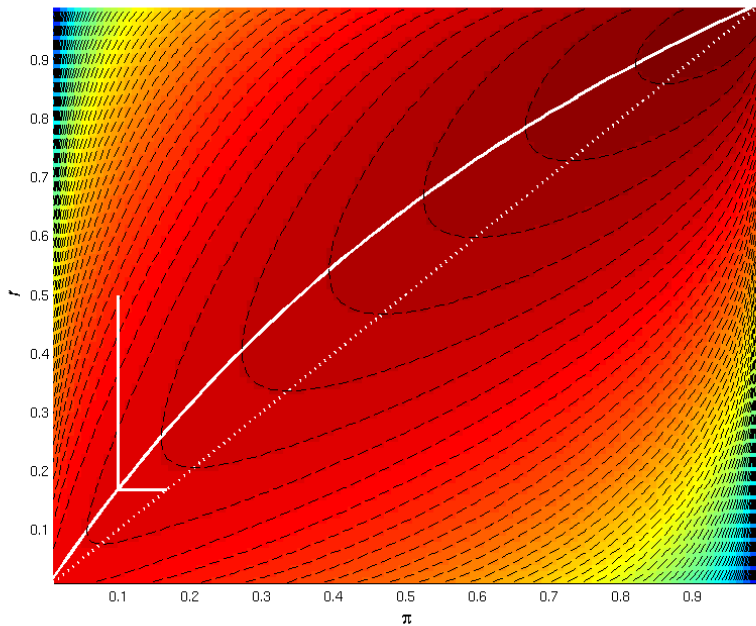
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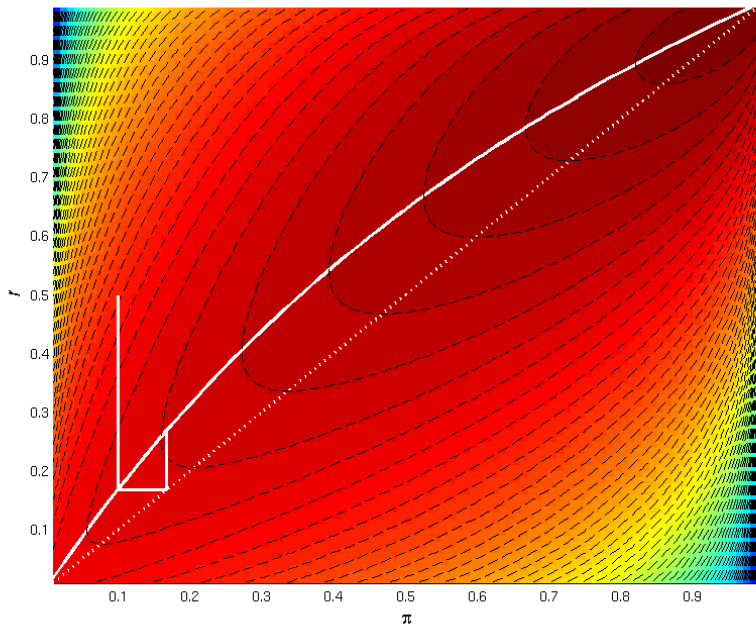
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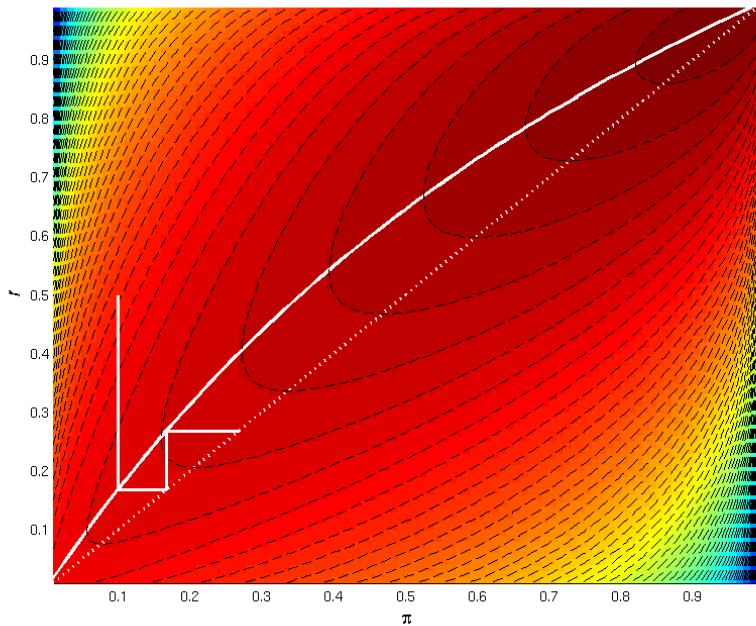
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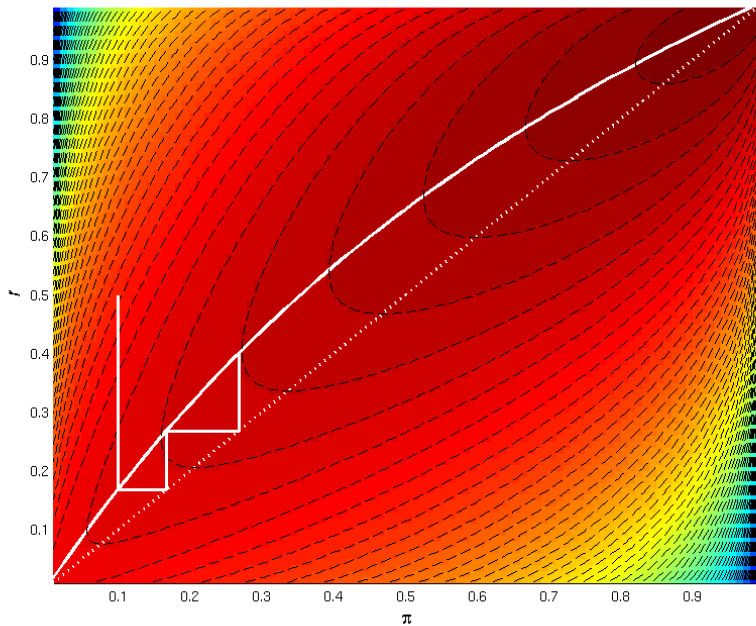
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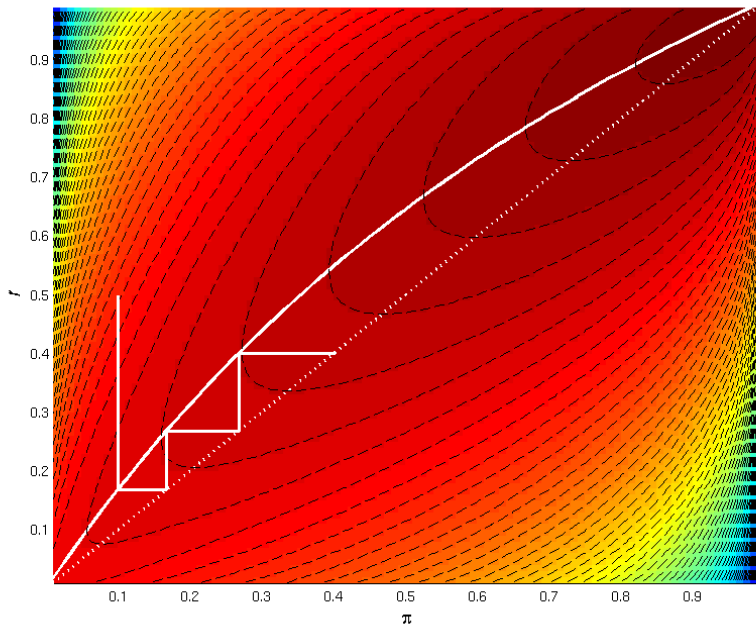
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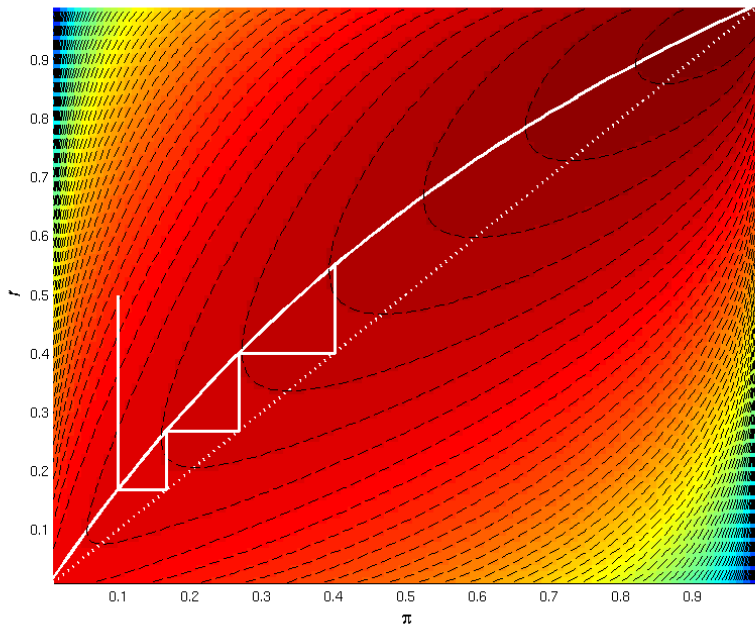
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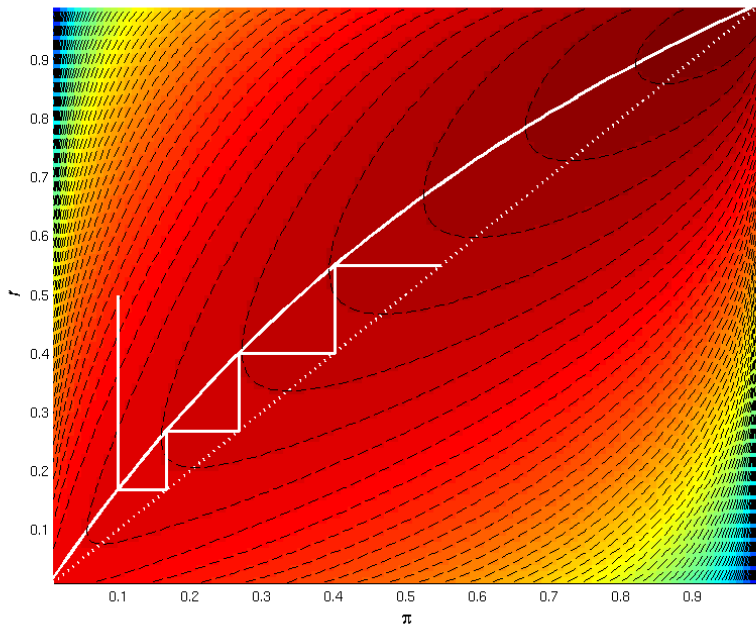
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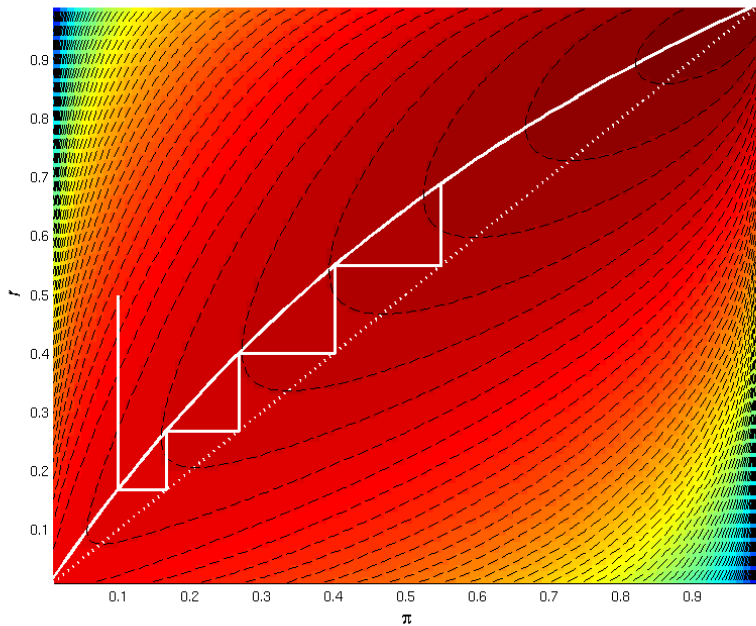
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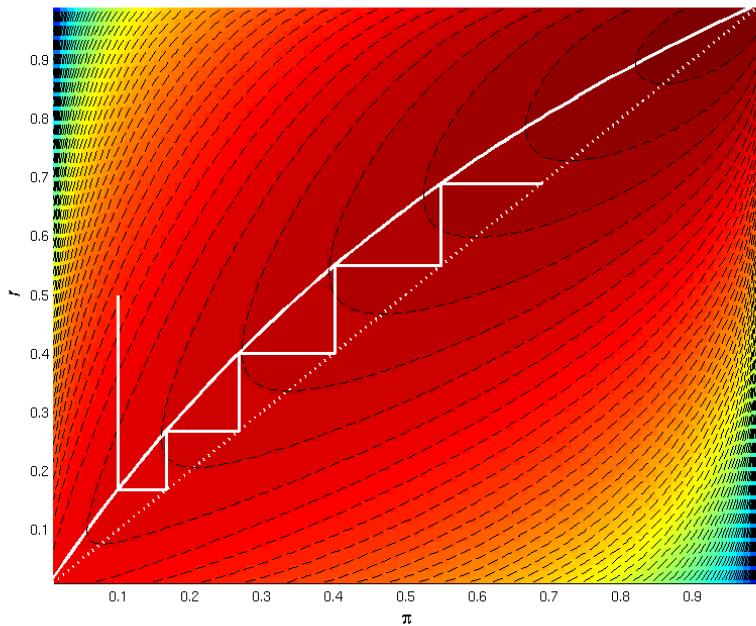
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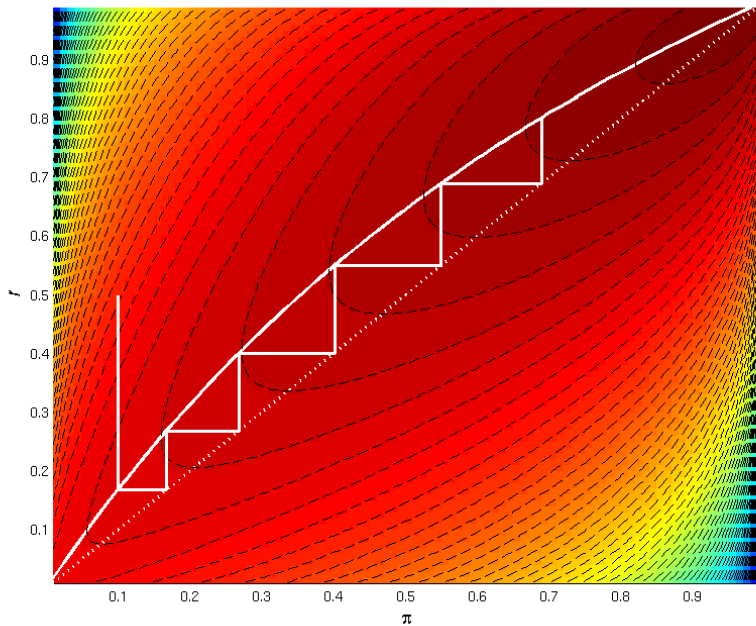
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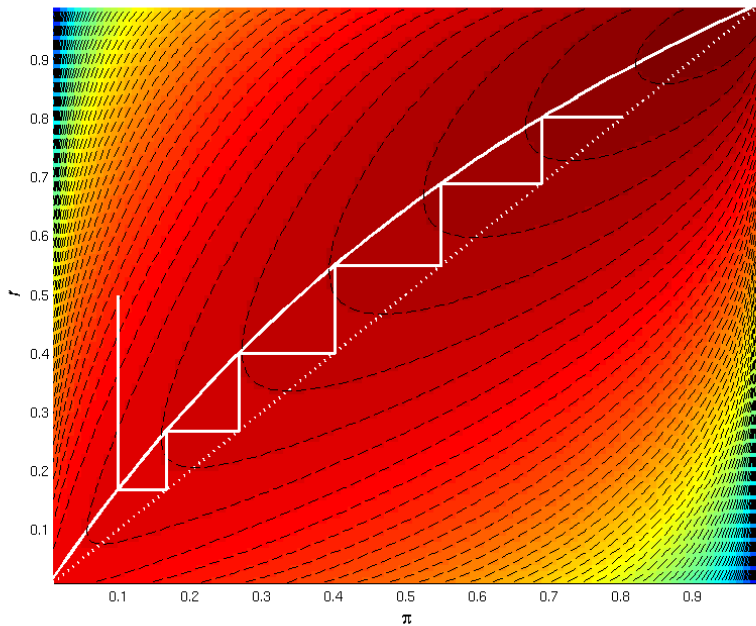
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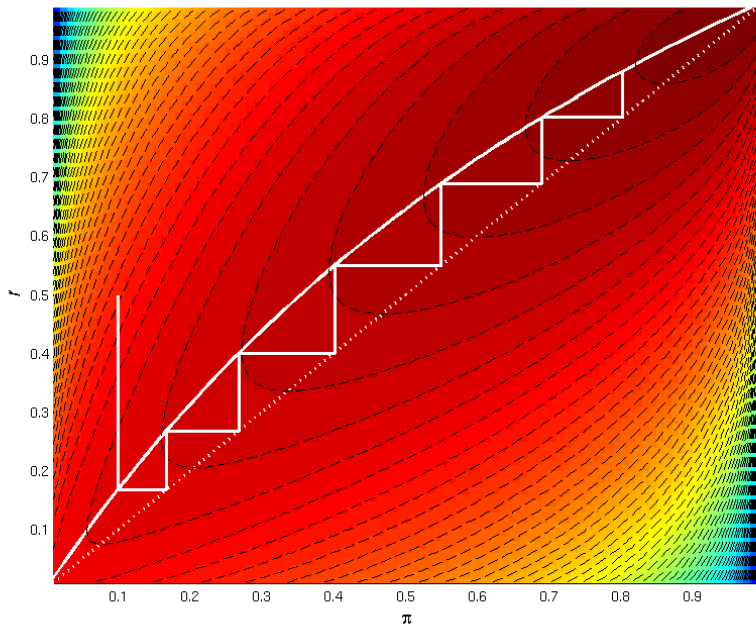
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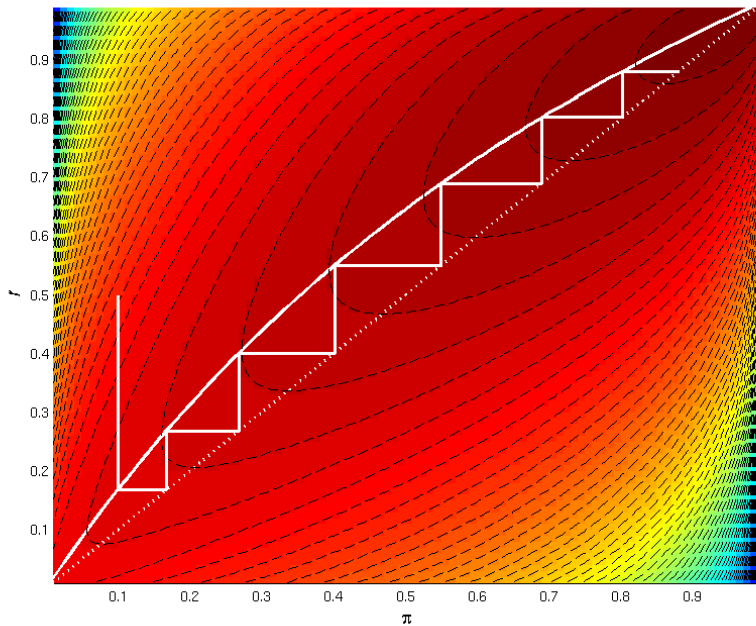
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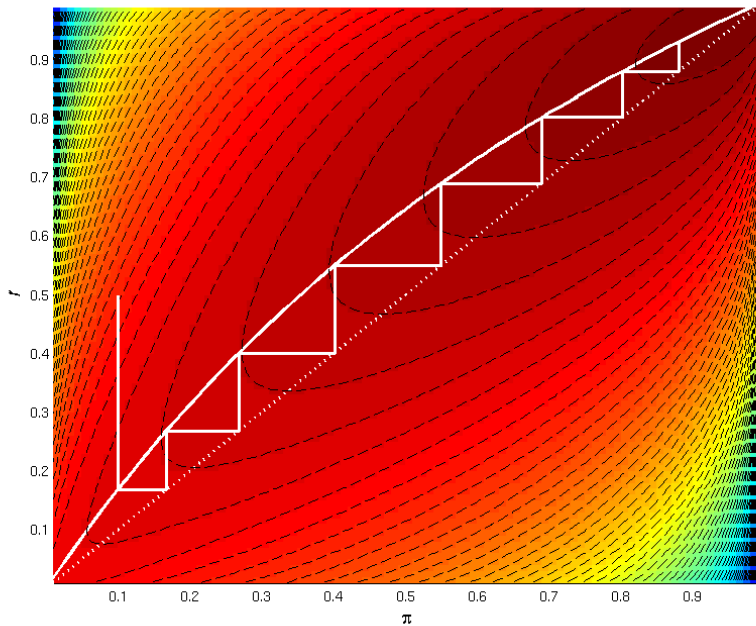
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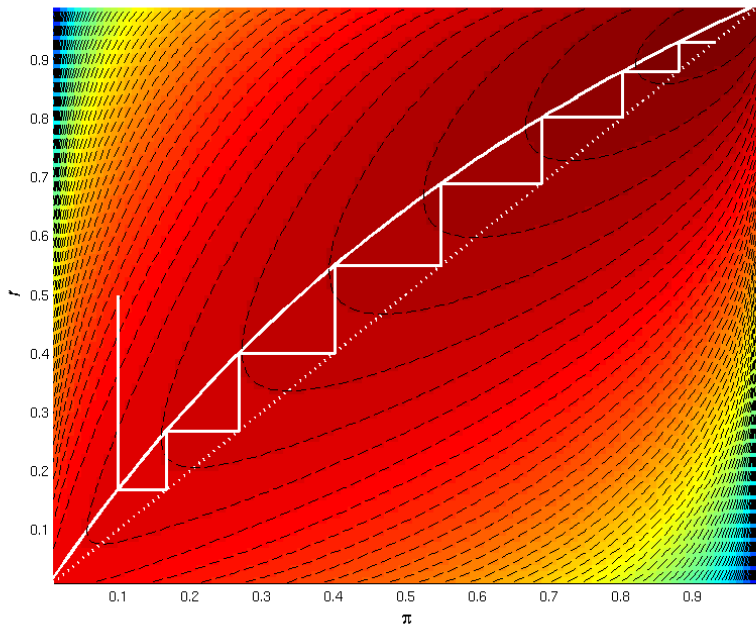
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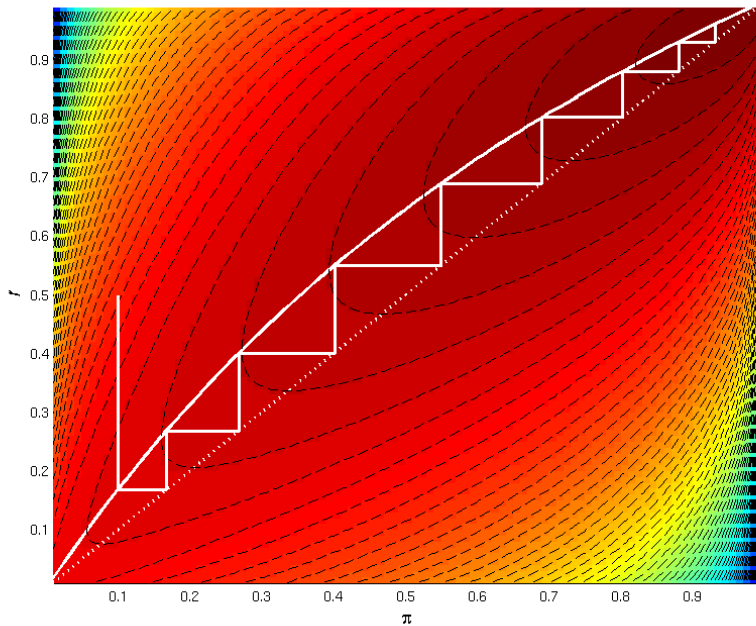
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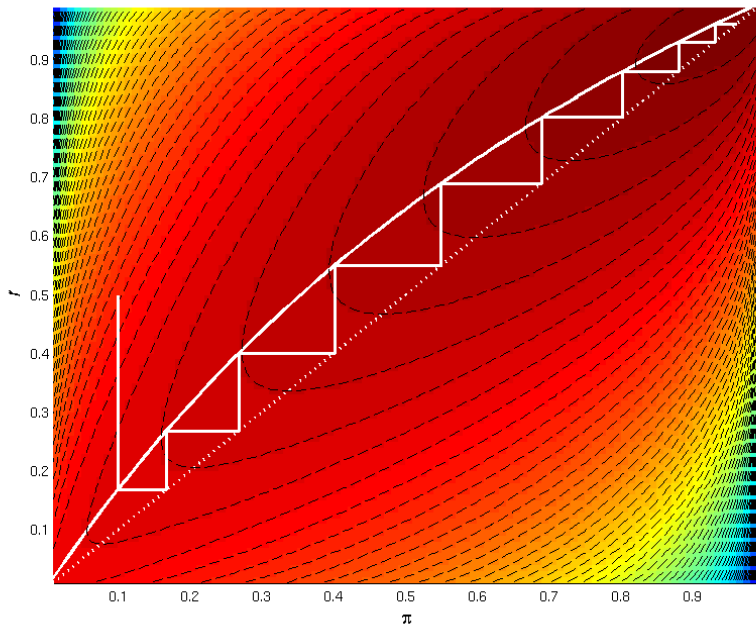
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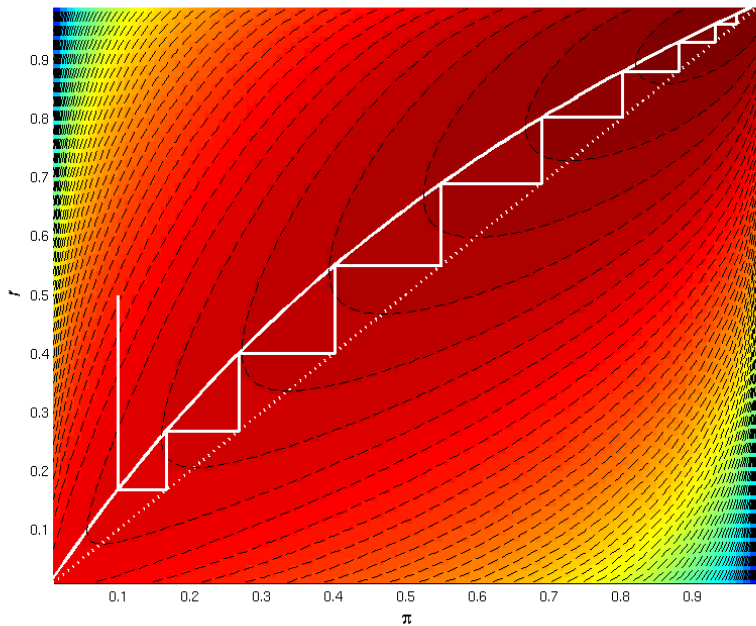
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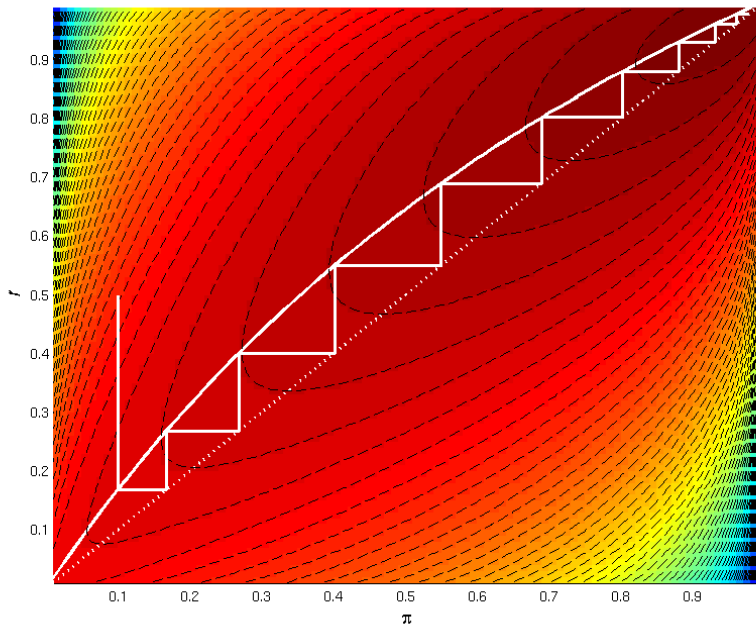
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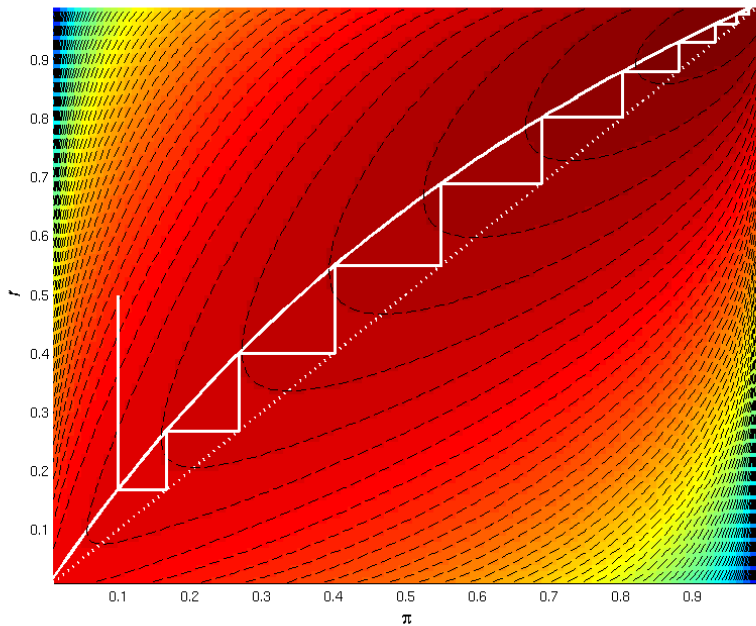
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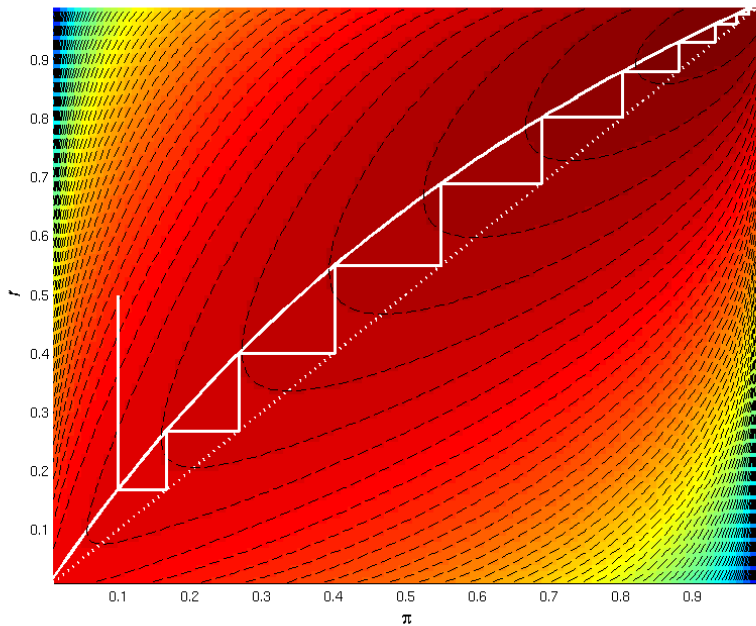
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Can also show that fixed points of EM (generally) correspond to maxima of the likelihood (see appendices).

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- ▶ 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

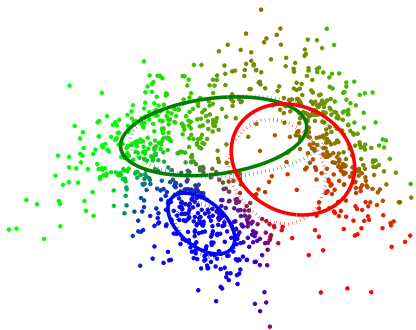
$$\left. \frac{\partial}{\partial \theta} \right|_{\theta^{(k-1)}} \langle \log P(\mathcal{X}, \mathcal{Y} | \theta) \rangle_{q^{(k)}(\mathcal{Y}) [= P(\mathcal{Y} | \mathcal{X}, \theta^{(k-1)})]} = \left. \frac{\partial}{\partial \theta} \right|_{\theta^{(k-1)}} \log P(\mathcal{X} | \theta)$$

[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 q_s .

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

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

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

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

The Gaussian mixture model (E-step)

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

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

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$$q(s_i = m) \propto \frac{\pi_m}{\sigma_m} \exp \left\{ -\frac{1}{2\sigma_m^2} (x_i - \mu_m)^2 \right\}$$

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

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):

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

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

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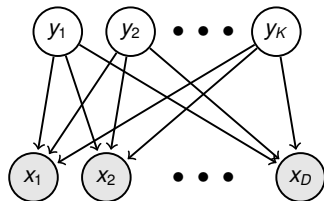
$$\begin{aligned} E &= \langle \log p(x, s|\theta) \rangle_{q(s)} = \sum q(s) \log[p(s|\theta) p(x|s, \theta)] \\ &= \sum_{i,m} r_{im} \left[\log \pi_m - \log \sigma_m - \frac{1}{2\sigma_m^2} (x_i - \mu_m)^2 \right]. \end{aligned}$$

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

EM for Factor Analysis



The model for \mathbf{x} :

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

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 $\mathcal{F}(q, \theta)$:

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

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 ?

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

So $\Sigma = (I + \Lambda^T\Psi^{-1}\Lambda)^{-1} = I - \beta\Lambda$ and $\boldsymbol{\mu}_n = \Sigma\Lambda^T\Psi^{-1}\mathbf{x}_n = \beta\mathbf{x}_n$. Where $\beta = \Sigma\Lambda^T\Psi^{-1}$.
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 $\mathcal{F} = \sum_n \langle \log p(\mathbf{y}_n | \theta) + \log p(\mathbf{x}_n | \mathbf{y}_n, \theta) \rangle_{q_n(\mathbf{y}_n)} + \mathbf{c}$

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

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

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

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

The M step for Factor Analysis

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

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

The M step for Factor Analysis

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

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

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

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

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

The M step for Factor Analysis (cont.)

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

The M step for Factor Analysis (cont.)

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

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

The M step for Factor Analysis (cont.)

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

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

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

The M step for Factor Analysis (cont.)

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

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

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

The M step for Factor Analysis (cont.)

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

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

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

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

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

The M step for Factor Analysis (cont.)

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

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

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

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

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

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

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

The M step for Factor Analysis (cont.)

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

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

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

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

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

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

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

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

The M step for Factor Analysis (cont.)

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

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

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

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

As $\Sigma \rightarrow 0$ these become the equations for ML linear regression

Mixtures of Factor Analysers

Simultaneous clustering and dimensionality reduction.

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

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. $\theta = \{\{\pi_k, \boldsymbol{\mu}_k, \Lambda_k\}_{k=1\dots K}, \Psi\}$

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

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

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

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 $\langle \delta_{s_n=m} \mathbf{y}_n \mathbf{y}_n^\top \rangle$.

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:

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

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

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

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We also have:

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

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

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 .

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

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Collecting the M component distributions' natural params into a matrix $\Theta = [\theta_m]$:

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

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

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where $\log \mathbf{Z}(\Theta)$ collects the log-normalisers for all components into an M -element vector. Then, the expected sufficient statistics (E-step) are:

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

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

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

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

EM for MAP

What if we have a prior?

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

$$p(\theta) = F(\nu, \boldsymbol{\tau}) \exp\{\theta^T \boldsymbol{\tau}\} / Z(\theta)^\nu$$

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Augment the free energy by adding the log prior:

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

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

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What if we have a prior?

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

Augment the free energy by adding the log prior:

$$\begin{aligned} \mathcal{F}_{\text{MAP}}(q, \theta) &= \int q(\mathcal{Y}) \log p(\mathcal{Y}, \mathcal{X}, \theta) d\mathcal{Y} + \mathbf{H}[q] \leq \log P(\mathcal{X}|\theta) + \log P(\theta) \\ &= \int q(\mathcal{Y}) [\theta^T (\sum_i \mathbf{T}(\mathbf{z}_i) + \boldsymbol{\tau}) - (N + \nu) \log Z(\theta)] d\mathcal{Y} + \text{const wrt } \theta \\ &= \theta^T (\langle \mathbf{T}(\mathbf{z}) \rangle_{q(\mathcal{Y})} + \boldsymbol{\tau}) - (N + \nu) \log Z(\theta) + \text{const wrt } \theta \end{aligned}$$

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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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”.

References

- ▶ A. P. Dempster, N. M. Laird and D. B. Rubin (1977).
Maximum Likelihood from Incomplete Data via the EM Algorithm. Journal of the Royal Statistical Society. Series B (Methodological), Vol. 39, No. 1 (1977), pp. 1-38.
<http://www.jstor.org/stable/2984875>
- ▶ R. M. Neal and G. E. Hinton (1998).
A view of the EM algorithm that justifies incremental, sparse, and other variants. In M. I. Jordan (editor) Learning in Graphical Models, pp. 355-368, Dordrecht: Kluwer Academic Publishers.
<http://www.cs.utoronto.ca/~radford/ftp/emk.pdf>
- ▶ R. Salakhutdinov, S. Roweis and Z. Ghahramani, (2003).
Optimization with EM and expectation-conjugate-gradient. In ICML (pp. 672-679).
<http://www.cs.utoronto.ca/~rsalakhu/papers/emecg.pdf>
- ▶ Z. Ghahramani and G. E. Hinton (1996).
The EM Algorithm for Mixtures of Factor Analyzers. University of Toronto Technical Report CRG-TR-96-1.
<http://learning.eng.cam.ac.uk/zoubin/papers/tr-96-1.pdf>

Proof of the Matrix Inversion Lemma

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

Need to prove:

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

Expand:

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

Regroup:

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

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:

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

Find conditions for stationarity

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

Check sign of curvature (Hessian):

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

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

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:

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

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