

Graphical Models, Inference and Learning

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Tutorial paper available at:
www.psi.toronto.edu/~frey/stuff/tutorial.ps.gz

Acknowledgements

- Nebojsa Jojic, Microsoft Research
- Resources:
 - Neal and Hinton 93, A new view of the EM algorithm
 - Jordan 98 (ed), Inference and Learning in Graphical Models
 - Wiberg, Loeliger, Koetter 95, The sum-product algorithm for error-correcting decoding
 - Neal 93, Probabilistic inference using Markov chain Monte Carlo techniques
 - ... (see tutorial paper)

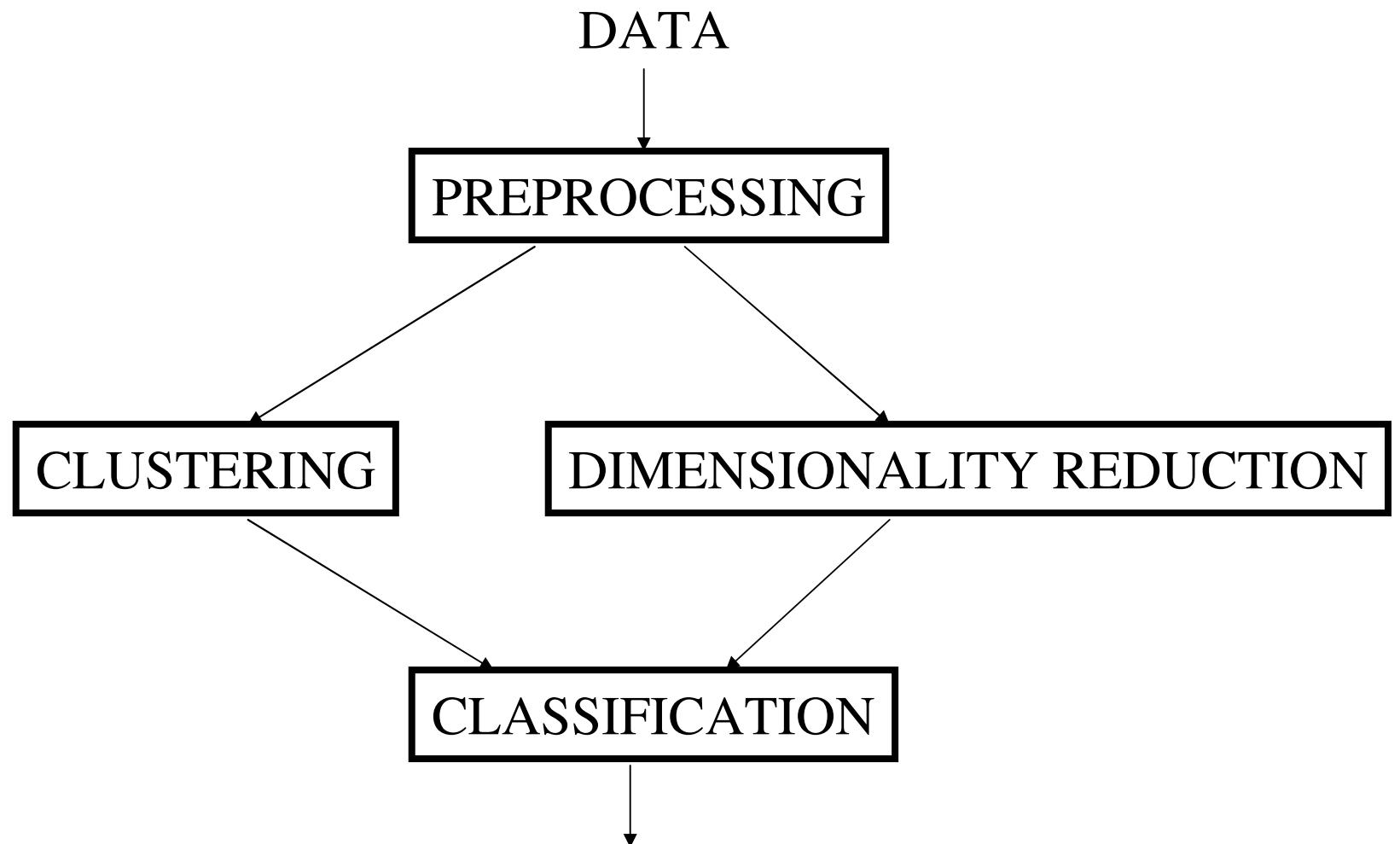
Motivation

- Computer vision
- Communications systems
- Molecular biology
- Microphone array processing
- ...

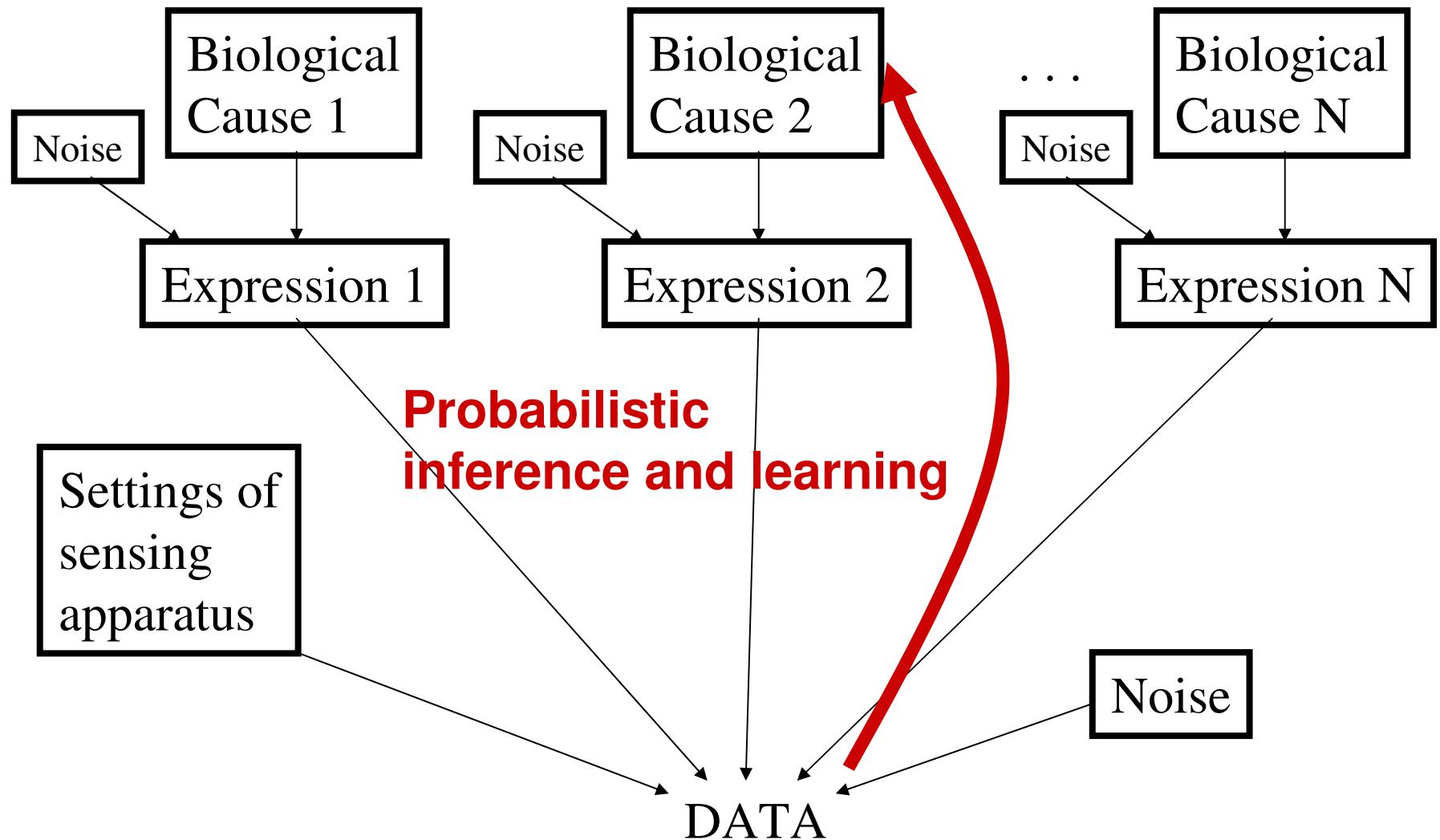
Discriminative models and Generative models

- Discriminative: $P(\text{class}|\text{input})$
 - Supervised learning
- Generative: $P(\text{class}, \text{input})$
 - Supervised or unsupervised learning (class unobserved)
- Hidden variables:
 - $P(\text{class}|\text{input}) = \sum_{\text{hidden}} P(\text{class}, \text{hidden}|\text{input})$
 - $P(\text{class}, \text{input}) = \sum_{\text{hidden}} P(\text{class}, \text{hidden}, \text{input})$

Sequential (block-diagram) data analysis



The generative approach (on a genomics problem)



Modularity and Graphical Models

- $P(\text{class}, \text{hidden}, \text{input})$ is complex for real-world problems
 - How do we specify constraints on variables?
 - How do we modify sub-components of the model?
 - How do we cope with computational intractability?
 - How do we cope with learnability?
- Graphical models: Modular descriptions of complex probability models

Case study: Occlusion Model

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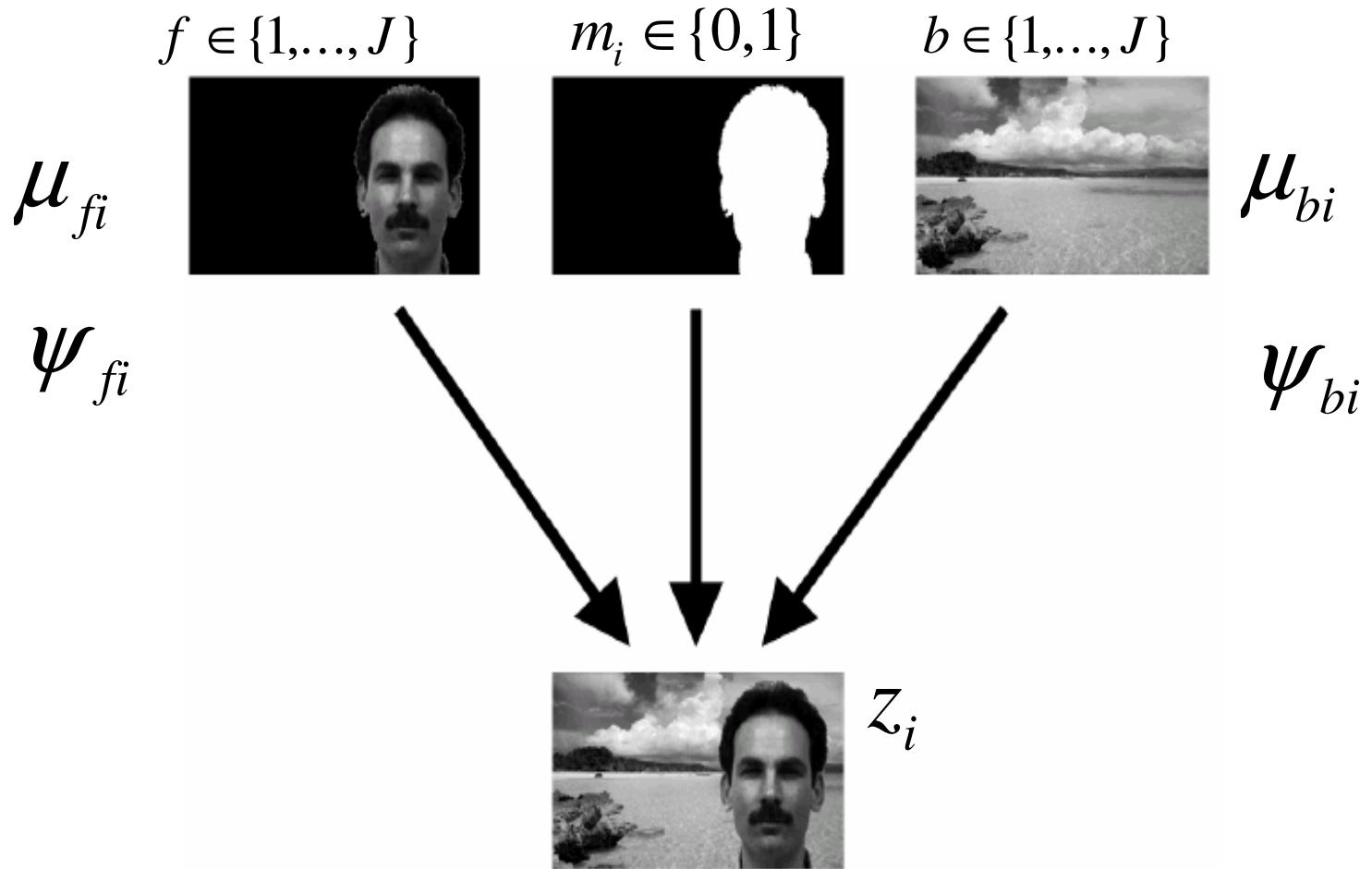
A sample from the dataset

(5 different faces against 7 different backgrounds)



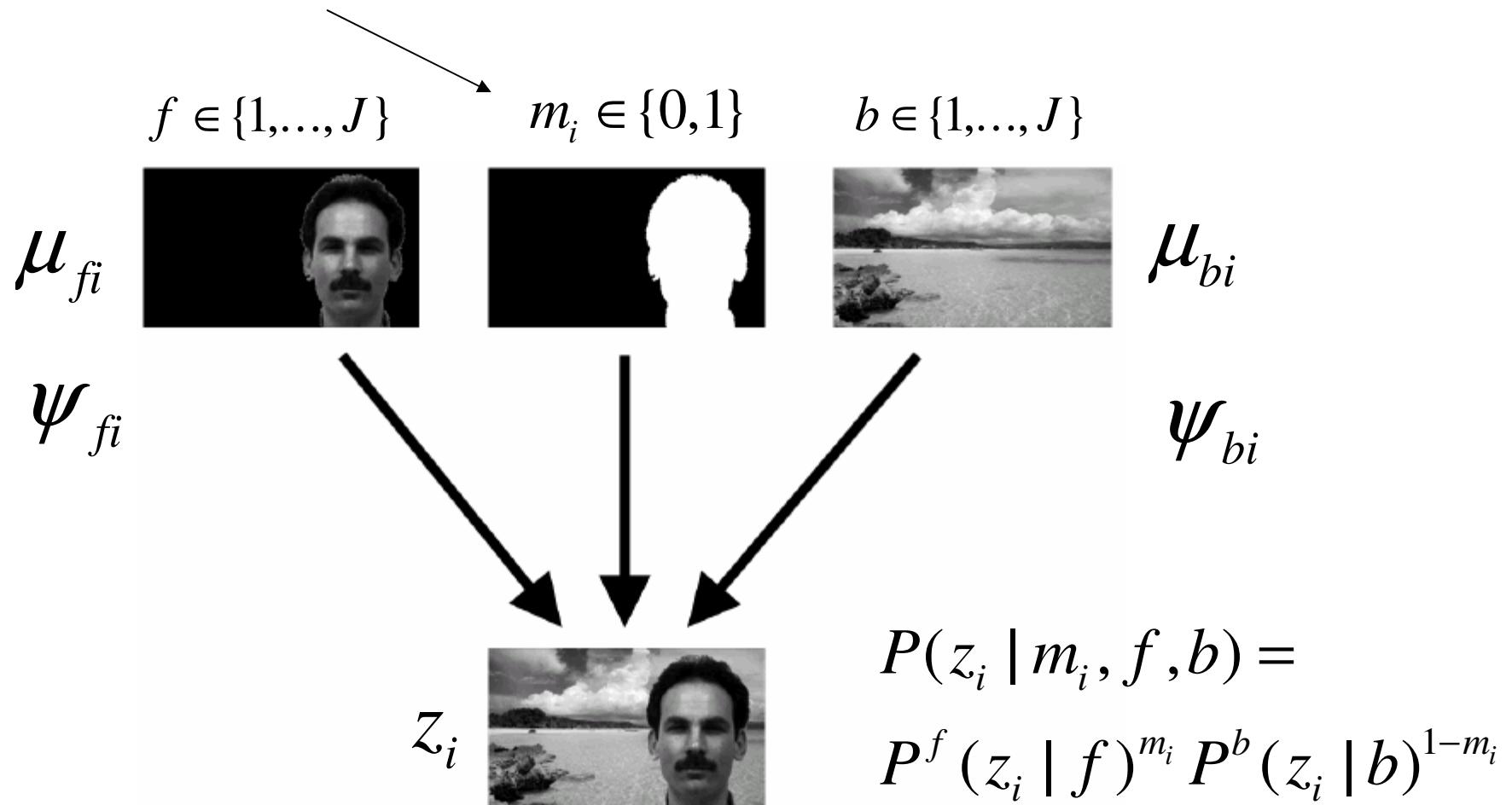
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Generative model



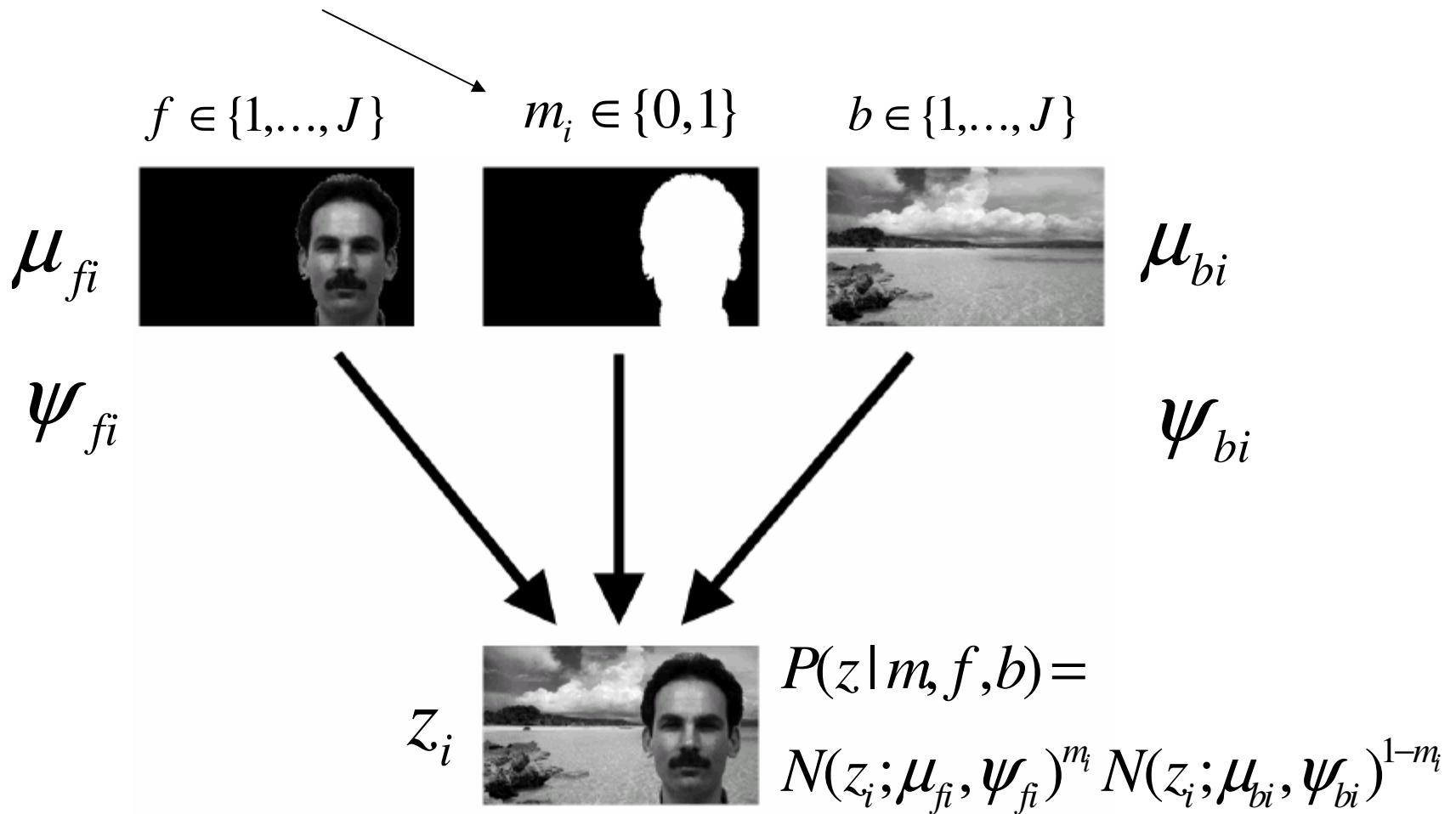
Let α_i be the probability that $m_i=1$ given that the foreground class is f ,

i.e., $P(m_i=1 | f) = \alpha_i$, $P(m_i=0 | f) = 1-\alpha_i$,



Let α_i be the probability that $m_i=1$ given that the foreground class is f ,

i.e., $P(m_i=1 | f) = \alpha_i$, $P(m_i=0 | f) = 1-\alpha_i$,



The joint probability distribution

$$P(z, m, f, b) = P(b)P(f)(\prod_{i=1}^K P(m_i | f))(\prod_{i=1}^K P(z_i | m_i, f, b)).$$

$$\alpha_i = P(m_i = 1 | f)$$

$$f \in \{1, \dots, J\}$$

$$m_i \in \{0, 1\}$$

$$b \in \{1, \dots, J\}$$

$$\mu_{fi}$$



$$\mu_{bi}$$

$$\psi_{fi}$$

$$\psi_{bi}$$



$$z_i$$

The joint probability distribution

$$P(z, m, f, b) = P(b)P(f)(\prod_{i=1}^K P(m_i | f))(\prod_{i=1}^K P(z_i | m_i, f, b))$$

Because m is binary, we can write:

$$P(z_i | m_i, f, b) = P^f(z_i | f)^{m_i} P^b(z_i | b)^{1-m_i}$$

$$P(z, m, f, b) = \pi_b \pi_f (\prod_{i=1}^K \alpha_{fi}^{m_i} (1 - \alpha_{fi})^{1-m_i} N(z_i; \mu_{fi}, \psi_{fi})^{m_i} N(z_i; \mu_{bi}, \psi_{bi})^{1-m_i}).$$

The diagram illustrates the components of the joint probability equation. Arrows point from labels to specific terms in the equation:

- An arrow points from "Prior distribution of foreground and background classes" to $\pi_b \pi_f$.
- An arrow points from "Probability of occlusion" to $(\prod_{i=1}^K \alpha_{fi}^{m_i} (1 - \alpha_{fi})^{1-m_i})$.
- An arrow points from "Mask at pixel i" to $N(z_i; \mu_{fi}, \psi_{fi})^{m_i}$.
- An arrow points from "Observed intensity of the pixel i" to $N(z_i; \mu_{bi}, \psi_{bi})^{1-m_i}$.
- An arrow points from "Means and variances of the layer classes" to both μ_{fi} , ψ_{fi} , μ_{bi} , and ψ_{bi} .

Joint distribution over all variables and parameters in the dataset

- We assume uniform prior over the parameters

$$P(\mu, \psi, \pi, \alpha, f^{(1)}, b^{(1)}, m^{(1)}, \dots, f^{(T)}, b^{(T)}, m^{(T)} | z^{(1)}, \dots, z^{(T)})$$

$$\propto \prod_{t=1}^T \left(\pi_{f(t)} \pi_{b(t)} \left(\prod_{i=1}^K \alpha_{f(t)i}^{m_i^{(t)}} (1 - \alpha_{f(t)i})^{1-m_i^{(t)}} \mathcal{N}(z_i^{(t)}; \mu_{f(t)i}, \psi_{f(t)i})^{m_i^{(t)}} \mathcal{N}(z_i^{(t)}; \mu_{b(t)i}, \psi_{b(t)i})^{1-m_i^{(t)}} \right) \right)$$

Inference

$$P(m, f, b \mid z) \propto \pi_b \pi_f \left(\prod_{i=1}^K \alpha_{fi}^{m_i} (1 - \alpha_{fi})^{1-m_i} N(z_i; \mu_{fi}, \psi_{fi})^{m_i} N(z_i; \mu_{bi}, \psi_{bi})^{1-m_i} \right).$$

$$P(m, f, b \mid z) = P(f, b \mid z) P(m \mid f, b, z) = P(f, b \mid z) \prod_{i=1}^K P(m_i \mid f, b, z).$$

$$\begin{aligned} P(f, b \mid z) &\propto P(f, b, z) = \sum_{m_1} \cdots \sum_{m_K} P(m, f, b, z) \\ &= \pi_b \pi_f \prod_{i=1}^K (\alpha_{fi} N(z_i; \mu_{fi}, \psi_{fi}) + (1 - \alpha_{fi}) N(z_i; \mu_{bi}, \psi_{bi})). \end{aligned}$$

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Bayesian Networks

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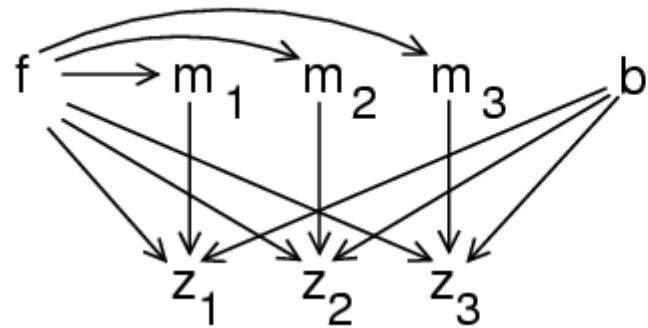
Bayesian network

- MAY be constructed using knowledge of causal relationships
- Quickly conveys the factorization of a distribution
- Clearly expresses dependencies and independencies between variables
- Can be used to derive fast inference algorithms

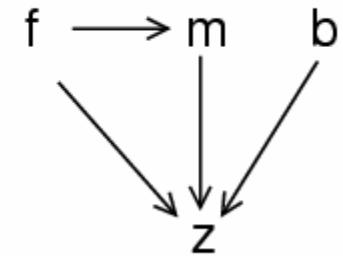
Bayes net for occlusion model

$$P(z, m, f, b) = P(b)P(f)(\prod_{i=1}^K P(m_i | f))(\prod_{i=1}^K P(z_i | m_i, f, b))$$

(a)

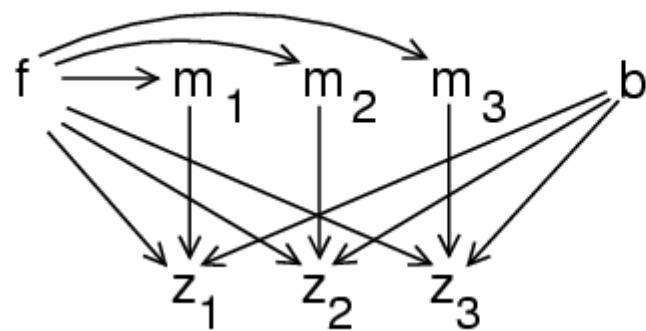


(b)

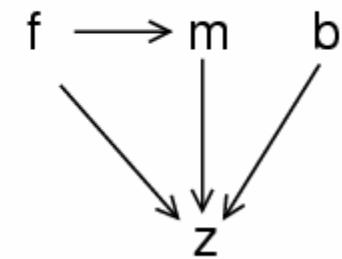


Simulating Bayes nets

(a)

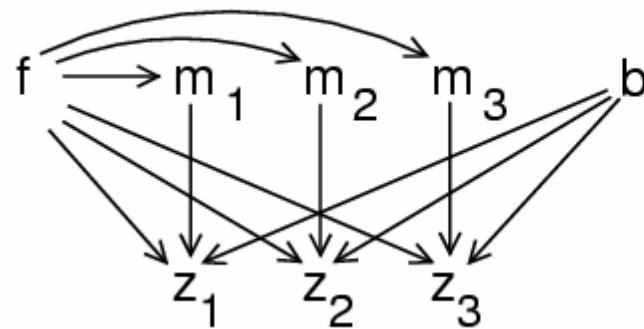


(b)

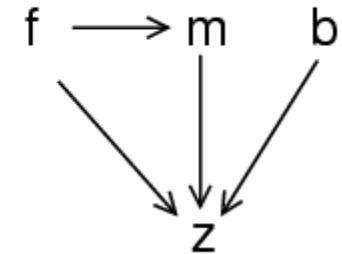


Conditional independence

(a)



(b)



A greedy inference and learning algorithm: ICM

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Iterative Conditional Modes (ICM)

- For $t = 1, \dots, T$

$$\{ f^{(t)} \leftarrow \operatorname{argmax}_{f^{(t)}} [\pi_{f^{(t)}} \prod_{i:m_i^{(t)}=1} \mathcal{N}(z_i^{(t)}; \mu_{f^{(t)}i}, \psi_{f^{(t)}i})]$$

$$\{ b^{(t)} \leftarrow \operatorname{argmax}_{b^{(t)}} [\pi_{b^{(t)}} \prod_{i:m_i^{(t)}=0} \mathcal{N}(z_i^{(t)}; \mu_{b^{(t)}i}, \psi_{b^{(t)}i})]$$

$$\{ \text{For } i = 1, \dots, K: m_i^{(t)} \leftarrow \begin{cases} 1 & \text{if } \alpha_{f^{(t)}i} \mathcal{N}(z_i^{(t)}; \mu_{f^{(t)}i}, \psi_{f^{(t)}i}) > (1 - \alpha_{f^{(t)}i}) \mathcal{N}(z_i^{(t)}; \mu_{b^{(t)}i}, \psi_{b^{(t)}i}) \\ 0 & \text{otherwise} \end{cases}$$

- For $j = 1, \dots, J$

$$\{ \pi_j \leftarrow (\sum_{t=1}^T [f^{(t)} = j] + \sum_{t=1}^T [b^{(t)} = j]) / 2T$$

- For $j = 1, \dots, J$, for $i = 1, \dots, K$

$$\{ \alpha_{ji} \leftarrow (\sum_{t=1}^T [f^{(t)} = j] m_i^{(t)}) / (\sum_{t=1}^T [f^{(t)} = j])$$

$$\{ \mu_{ji} \leftarrow (\sum_{t=1}^T [f^{(t)} = j \text{ or } b^{(t)} = j] z_i^{(t)}) / (\sum_{t=1}^T [f^{(t)} = j \text{ or } b^{(t)} = j])$$

$$\{ \psi_{ji} \leftarrow (\sum_{t=1}^T [f^{(t)} = j \text{ or } b^{(t)} = j] (z_i^{(t)} - \mu_{ji})^2) / (\sum_{t=1}^T [f^{(t)} = j \text{ or } b^{(t)} = j])$$

Here, the Iverson notation is used where [True] = 1 and [False] = 0.

A sample from the dataset

(5 different faces against 7 different backgrounds)



Iterative model optimization

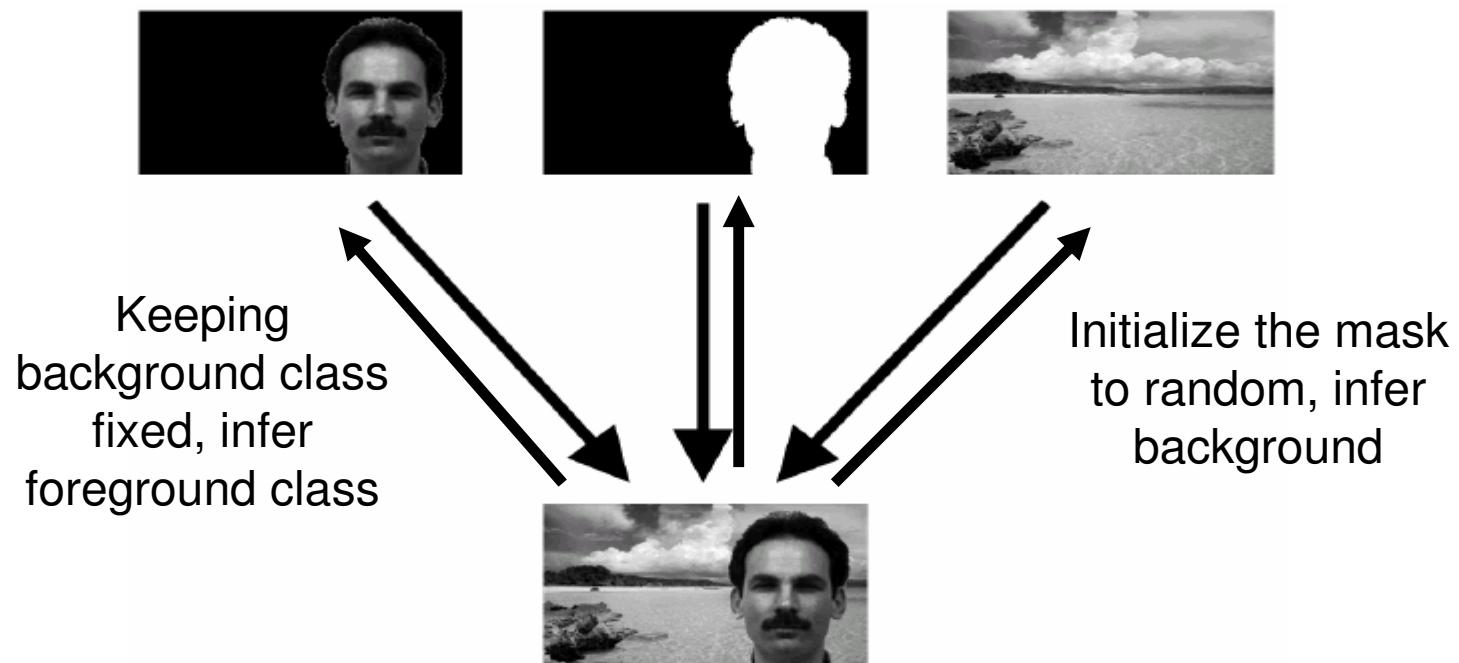
Two data samples



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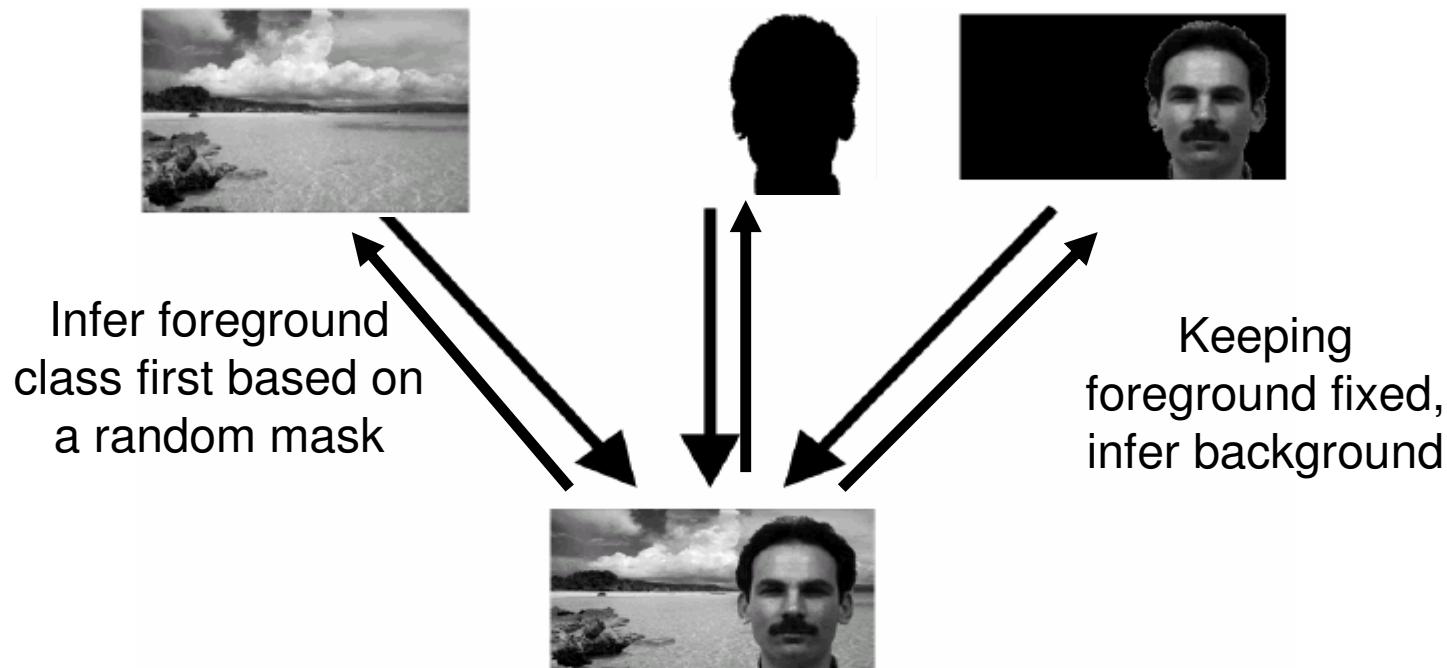
Inferring hidden variables using ICM

- Given the class means and variances and mask probabilities for each class, for the shown dataset, it is (sometimes) possible to invert the generative process

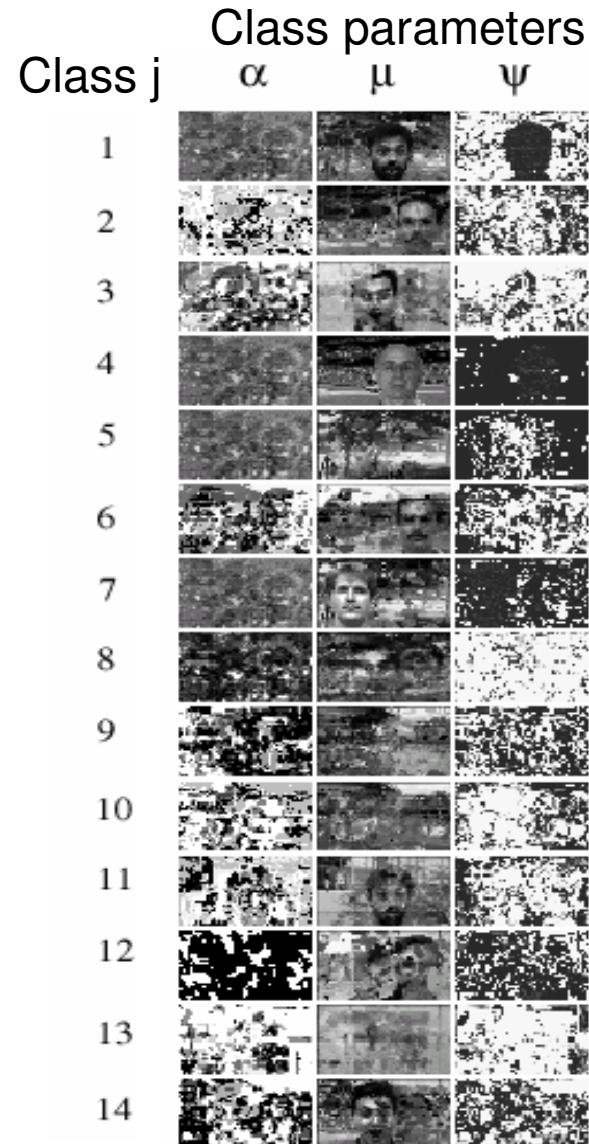


However...

- Order of updates is important



Inferring the hiddens *and* estimating the parameters of a 14-class model using ICM



ICM

- Simple, fast
- Prone to local maxima
- Can be seen as iteratively employing simplified conditional posteriors, e.g.,

$$P(m, f, b \mid z) \propto \pi_b \pi_f \prod_{i=1}^K \alpha_{fi}^{m_i} (1 - \alpha_{fi})^{1-m_i} N(z_i; \mu_{fi}, \psi_{fi})^{m_i} N(z_i; \mu_{bi}, \psi_{bi})^{1-m_i}$$

$$P(b \mid \hat{f}, \hat{m}, z) \propto \pi_b \pi_{\hat{f}} \prod_{i=1}^K \alpha_{\hat{f}i}^{\hat{m}_i} (1 - \alpha_{\hat{f}i})^{1-\hat{m}_i} N(z_i; \mu_{\hat{f}i}, \psi_{\hat{f}i})^{\hat{m}_i} N(z_i; \mu_{bi}, \psi_{bi})^{1-\hat{m}_i}$$

$$\hat{b} = \arg \max P(b \mid \hat{f}, \hat{m}, z)$$

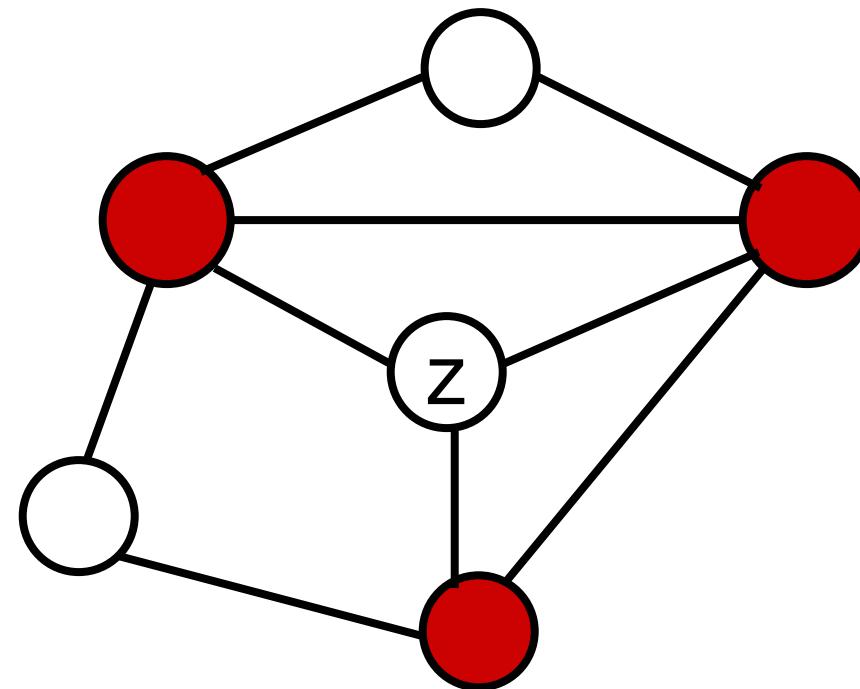
- Related to variational methods that use less severe approximations of the posterior

Markov Random Fields (MRFs)

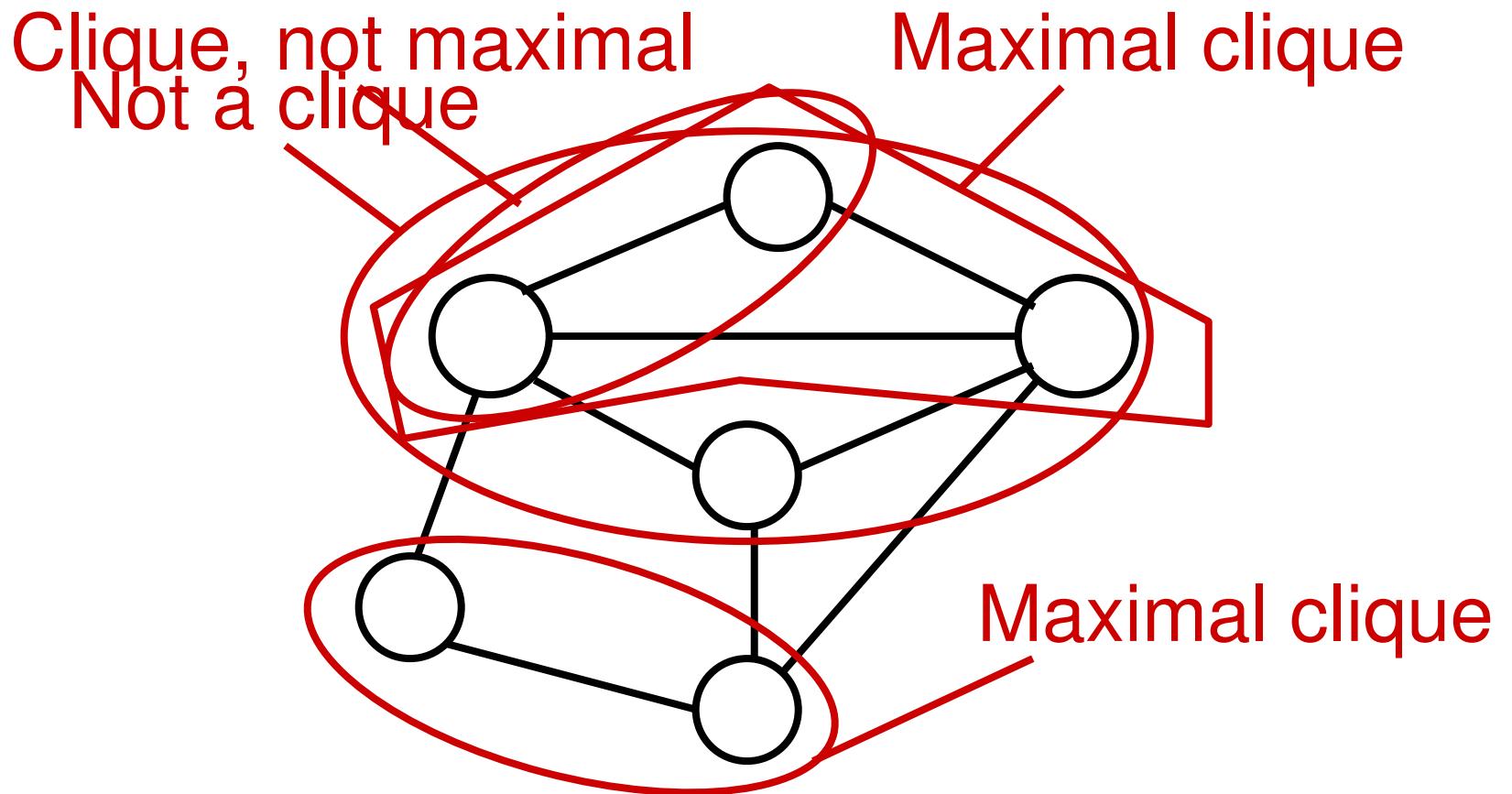
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Markov random fields (MRFs)

- Undirected graph on variables
- Each variable is independent of all other variables, given its neighbors



Cliques and maximal cliques



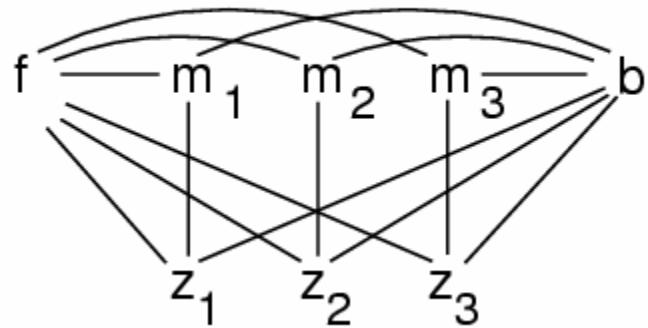
The distribution for an MRF

$$P(x_1, \dots, x_N) = \alpha \prod_i \Psi_i(x_{C_i})$$

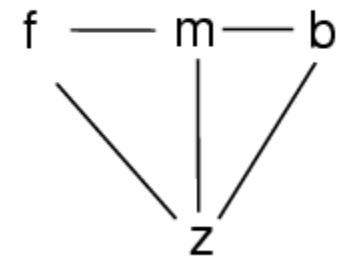
- i = index of maximal clique
 - C_i = set of indices of variables
 - x_{C_i} = set of variables
- $\Psi_i(x_{C_i})$ is a “potential” (“local function”)
- α is a normalizing constant

Occlusion model

(c)



(d)



$$P(z, m, f, b) = P(b)P(f)\left(\prod_{i=1}^K P(m_i \mid f)\right)\left(\prod_{i=1}^K P(z_i \mid m_i, f, b)\right).$$

Factor Graphs

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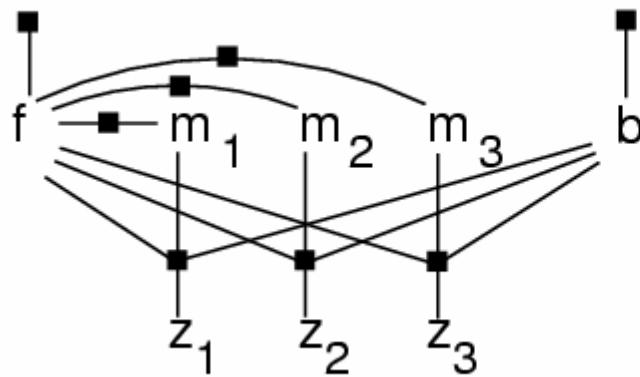
Factor graphs

(Kschischang, Frey and Loeliger, 1999)

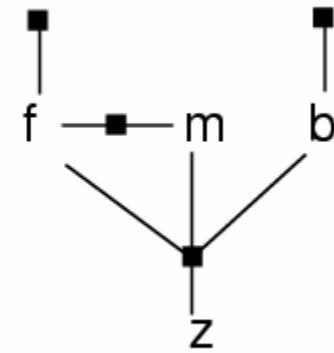
- Bipartite graph: nodes for variables and functions
- A *potential (local function)* is associated with each function node – this function depends on the neighboring variables
- The joint distribution is given by the product of the local functions
- Edges can be directed or undirected (a directed edge indicates a conditional probability)

Occlusion model

(e)



(f)



$$P(z, m, f, b) = P(b)P(f)(\prod_{i=1}^K P(m_i | f))(\prod_{i=1}^K P(z_i | m_i, f, b)).$$

Parameterized Models and Bayesian Learning

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Parameters as variables

- Recall for our toy problem:

$$P(z, m, f, b) = \pi_b \pi_f \left(\prod_{i=1}^K \alpha_{fi}^{m_i} (1 - \alpha_{fi})^{1-m_i} N(z_i; \mu_{fi}, \psi_{fi})^{m_i} N(z_i; \mu_{bi}, \psi_{bi})^{1-m_i} \right).$$

- Interpret the parameters as variables, where the joint distribution is

$$P(z, m, f, b, \pi, \alpha, \mu, \psi) = P(b | \pi) P(f | \pi) P(m | f, \alpha) P(z | m, f, b, \mu, \psi) P(\pi) P(\alpha) P(\mu) P(\psi).$$

where

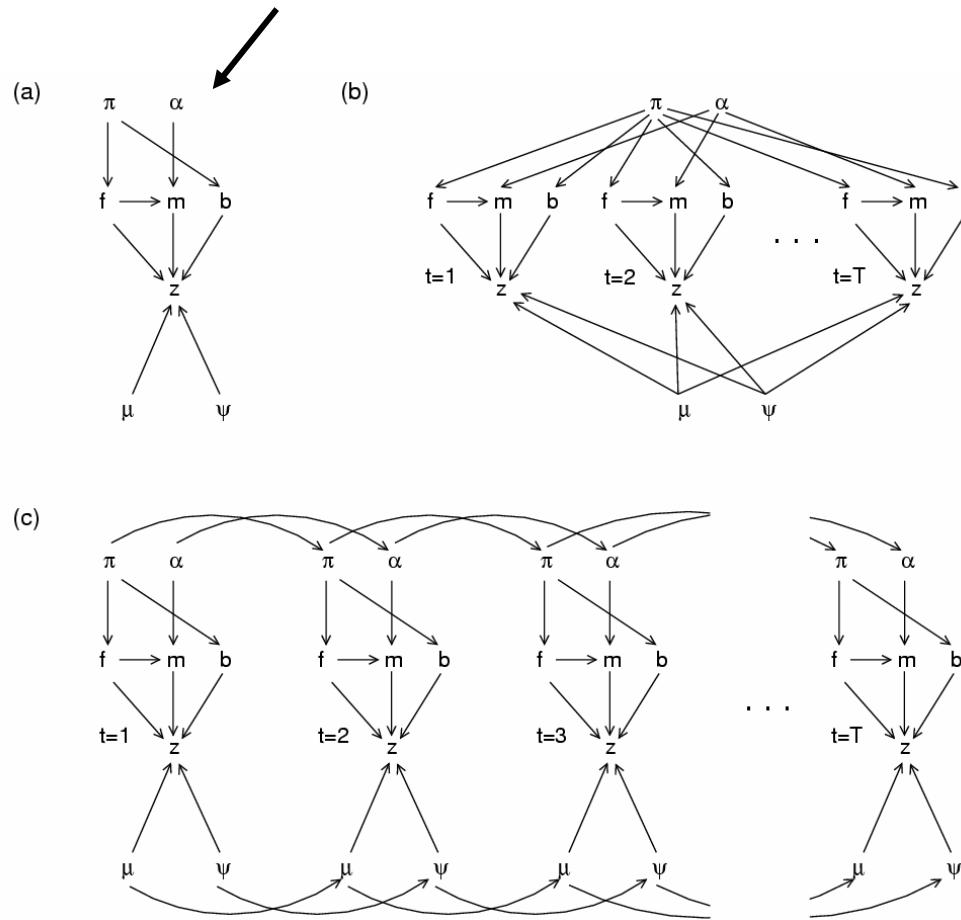
$$P(b | \pi) = \pi_b \quad P(f | \pi) = \pi_f \quad P(m_i | f, \alpha_{1i}, \dots, \alpha_{Ji}) = \alpha_{fi}^{m_i} (1 - \alpha_{fi})^{1-m_i}$$

$$P^f(z_i | f, \mu_{1i}, \dots, \mu_{Ji}, \psi_{1i}, \dots, \psi_{Ji}) = N(z_i; \mu_{fi}, \psi_{fi})$$

$$P^b(z_i | b, \mu_{1i}, \dots, \mu_{Ji}, \psi_{1i}, \dots, \psi_{Ji}) = N(z_i; \mu_{bi}, \psi_{bi})$$

Bayes nets for Bayesian version of toy problem

$$P(z, m, f, b, \pi, \alpha, \mu, \psi) = P(b | \pi)P(f | \pi)P(m | f, \alpha)P(z | m, f, b, \mu, \psi)P(\pi)P(\alpha)P(\mu)P(\psi).$$



Introducing training data

- **Visible variables:** $v = (v^{(1)}, \dots, v^{(T)})$
 - (t) denotes the t^{th} training case
- **Hidden variables:** $h = (h^\theta, h^{(1)}, \dots, h^{(T)})$
 - Parameters: h^θ
 - Variables for the t^{th} training case: $h^{(t)}$
- **Joint distribution:** $P(h, v) = P(h^\theta) \prod_{t=1}^T P(h^{(t)}, v^{(t)} | h^\theta).$
- **Parameter prior:** $P(h^\theta)$
- **Parameter likelihood:** $\prod_{t=1}^T P(h^{(t)}, v^{(t)} | h^\theta)$

Parameter priors

- Uniform priors
 - Computationally attractive
 - Problem: “Uniform” is inconsistent w.r.t. reparameterization
- Conjugate priors
 - Prior x Likelihood has same form as likelihood
 - Conjugate prior can be thought of as likelihood for “fake” data, eg, prior counts in a coin toss experiment

Algorithms for Inference and Learning

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Problem set-up

- Probabilistic inference and learning entail computing the intractable distribution,

$$P(h | v) = \frac{P(h, v)}{\int_h P(h, v)},$$

- Note that w.r.t. h , $P(h | v) \propto P(h, v)$.
- In a graphical model, $P(h, v)$ factorizes

General “brute force” inference

- Suppose x_1, x_2, \dots, x_N are binary

$$P(x_1) = \sum_{x_2} \sum_{x_3} \dots \sum_{x_N} P(x_1, x_2, \dots, x_N)$$

- This takes about 2^N operations
- Generally, computing $P(x_i | \text{Observed } x's)$ takes $2^{(N - \# \text{observed } x's)}$ operations

Exact posterior for occlusion model

$$P(\mu, \psi, \pi, \alpha, f^{(1)}, b^{(1)}, m^{(1)}, \dots, f^{(T)}, b^{(T)}, m^{(T)} | z^{(1)}, \dots, z^{(T)})$$

$$\propto \prod_{t=1}^T \left(\pi_{f(t)} \pi_{b(t)} \left(\prod_{i=1}^K \alpha_{f(t)i}^{m_i^{(t)}} (1 - \alpha_{f(t)i})^{1-m_i^{(t)}} \mathcal{N}(z_i^{(t)}; \mu_{f(t)i}, \psi_{f(t)i})^{m_i^{(t)}} \mathcal{N}(z_i^{(t)}; \mu_{b(t)i}, \psi_{b(t)i})^{1-m_i^{(t)}} \right) \right)$$

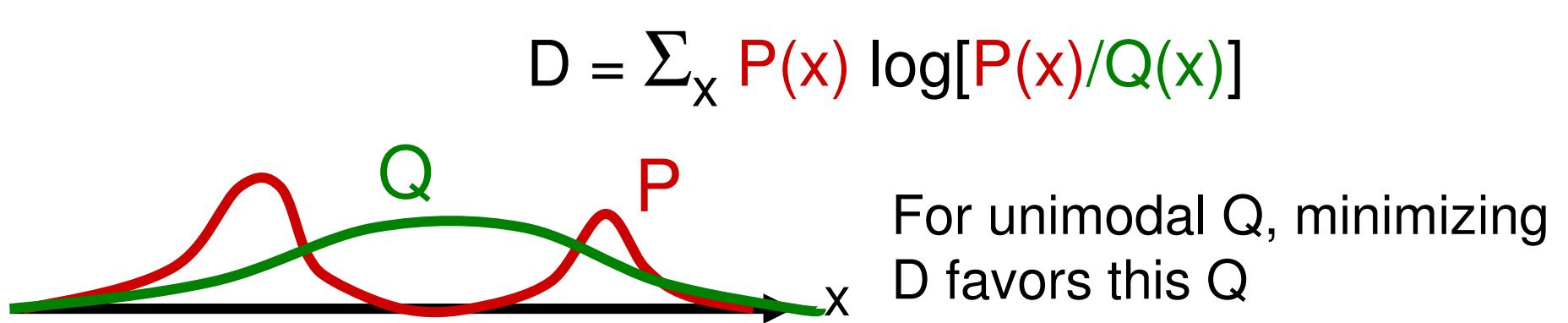
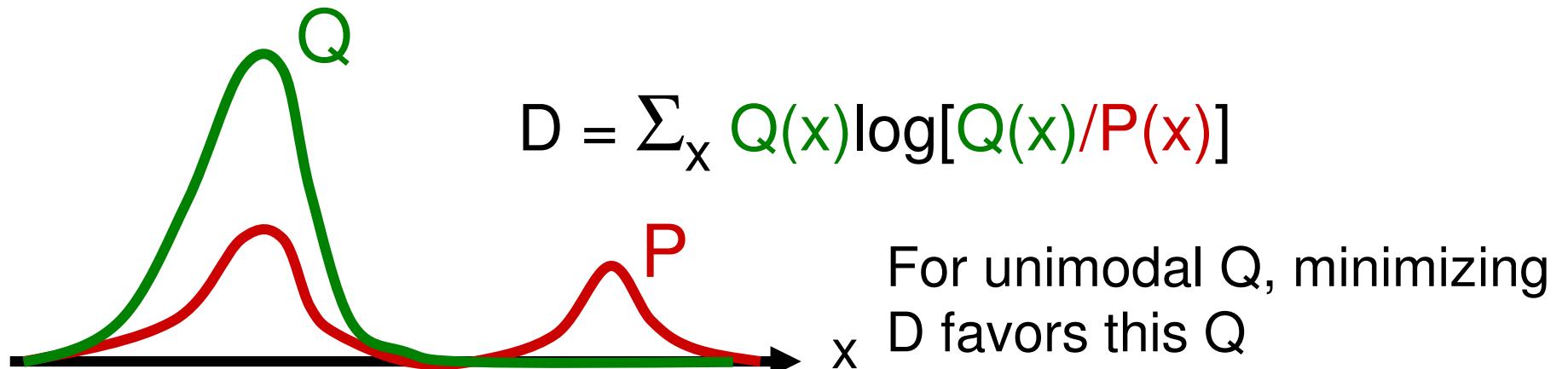
Approximate inference

- Since $P(h|v)$ is intractable, we search for a surrogate, $Q(h)$ that is tractable
- Measure of quality of Q : Kullback-Leibler divergence between Q and P ,

$$D(Q, P) = \int_h Q(h) \log \frac{Q(h)}{P(h | v)}.$$

- Properties:
 - $D \geq 0$
 - $D = 0$ iff $Q(h) = P(h|v)$

More on the “distance”



Free energy

- In fact, D is intractable
- We can make it tractable by subtracting $\log P(v)$

$$F(Q, P) = D(Q, P) - \log P(v)$$

$$= \int_h Q(h) \log \frac{Q(h)}{P(h | v)} - \int_h Q(h) \log P(v)$$

$$= \int_h Q(h) \log \frac{Q(h)}{P(h | v)P(v)}$$

$$= \int_h Q(h) \log \frac{Q(h)}{P(h, v)}.$$

Factorizes, for
a graphical model

Alternative derivation of free energy

- $\log P(v)$ is the log-likelihood of the data
- Computing $\log P(v)$ is intractable, but we can bound it using Jensen's inequality:

$$\begin{aligned}\log P(v) &= \log\left(\int_h P(h, v)\right) \\ &= \log\left(\int_h Q(h) \frac{P(h, v)}{Q(h)}\right) \\ &\geq \int_h Q(h) \log\left(\frac{P(h, v)}{Q(h)}\right) = -F(Q, P).\end{aligned}$$

Properties of free energy

- $F \geq -\log P(v)$
- The minimum of F w.r.t Q gives

$$F = -\log P(v)$$

$$Q(h) = P(h|v)$$

Approaches to constructing Q

- Parameterize Q directly
 - Iterative conditional modes
 - Variational methods (mean field)
 - Structured variational methods
 - Hybrids (the EM algorithm)
- Parameterize marginals of Q
 - Bethe approximation (probability propagation)
 - Kikuchi approximation (generalized prob prop)
- Represent Q using samples
 - Monte Carlo
 - Markov chain Monte Carlo

I.I.D. Training cases

Free energy for i.i.d. training cases

From (5), for a training set of T i.i.d. training cases with hidden variables $h = (h^\theta, h^{(1)}, \dots, h^{(T)})$ and visible variables $v = (v^{(1)}, \dots, v^{(T)})$, we have $P(h, v) = P(h^\theta) \prod_{t=1}^T P(h^{(t)}, v^{(t)} | h^\theta)$. The free energy is

$$\begin{aligned} F(Q, P) &= \int_h Q(h) \log Q(h) - \int_h Q(h) \log P(h, v) \\ &= \int_h Q(h) \log Q(h) - \int_{h^\theta} Q(h^\theta) \log P(h^\theta) - \sum_{t=1}^T \int_{h^{(t)}, h^\theta} Q(h^{(t)}, h^\theta) \log P(h^{(t)}, v^{(t)} | h^\theta). \end{aligned} \quad (8)$$

The decomposition of F into a sum of one term for each training case simplifies learning.

Point inference

- Discrete hidden variables: \hat{h} is a point estimate

$$F(Q, P) = \sum_h [h = \hat{h}] \log \frac{[h = \hat{h}]}{P(h, v)} = -\log P(\hat{h}, v).$$

– Minimizing F w.r.t. \hat{h} Maximizes $P(\hat{h}, v)$ w.r.t. h

- Continuous hidden variables:

$$F(Q, P) = \int_h \delta(h - \hat{h}) \log \frac{\delta(h - \hat{h})}{P(h, v)} = -\log P(\hat{h}, v) - H_\delta,$$

– Very common in engineering and science
– Problem: $H_\delta \rightarrow -\infty$

Iterative Conditional Modes (ICM)

Initialization. Pick values for all hidden variables h (randomly, or cleverly).

ICM Step. Select one of the hidden variables, h_i . Holding all other variables constant, set h_i to its MAP value:

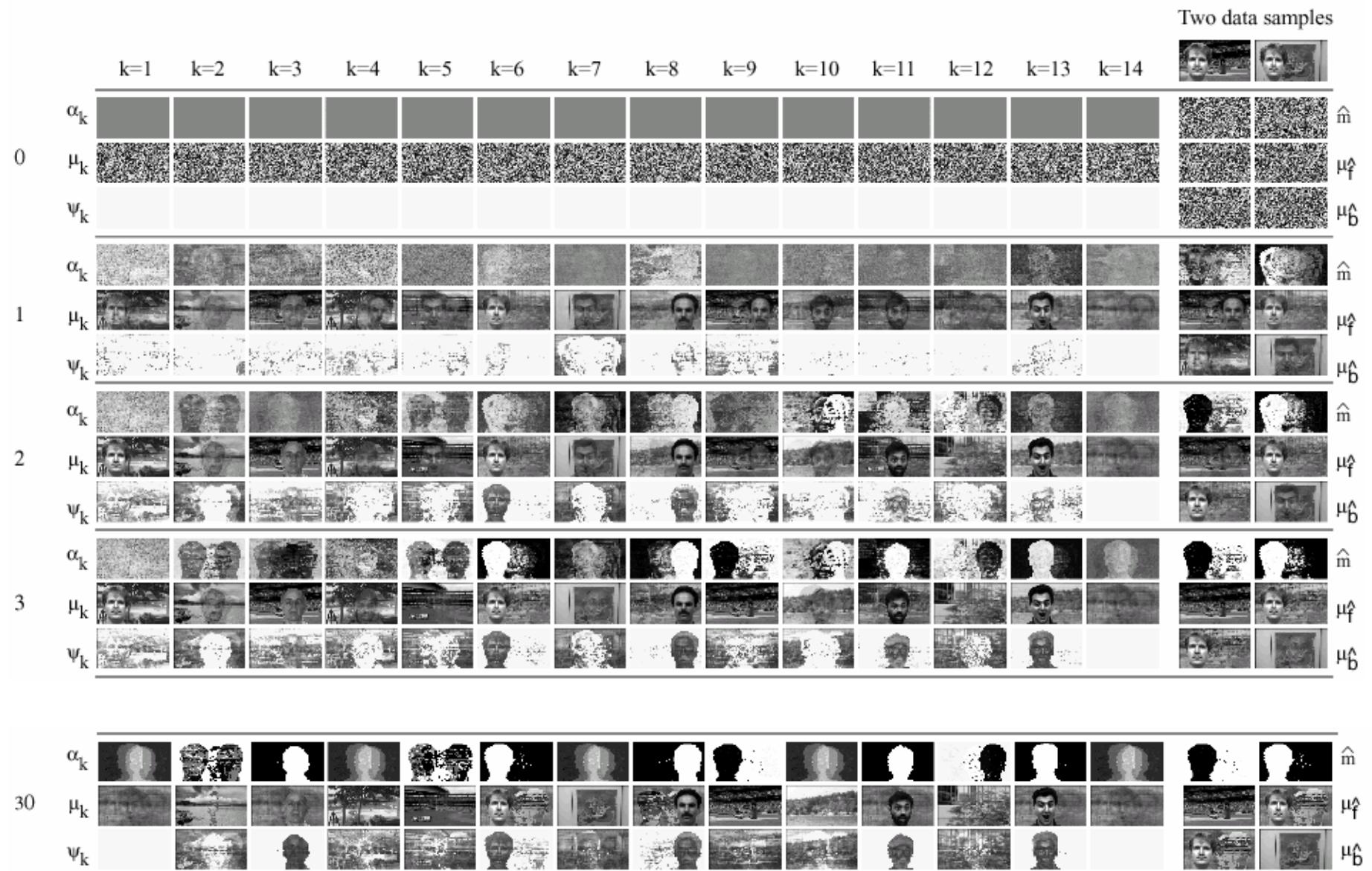
$$h_i \leftarrow \operatorname{argmax}_{h_i} P(h_i | h \setminus h_i, v) = \operatorname{argmax}_{h_i} P(h, v),$$

where $h \setminus h_i$ is the set of all hidden variables other than h_i .

Repeat for a fixed number of iterations or until convergence.

- Examples
 - ICM in mixture of Gaussians = k-means clustering
 - Clever ICM in M of G = sequential k-means clustering

Recall ICM for occlusion model



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Properties of ICM

- Fast, greedy
- Can get stuck in local minima
- Does not account for mass of mode
- Does not account for multiple modes
- Speed depends on choice of substructures
- Usually easy to implement

The EM Algorithm

- Use the following Q-distribution:

$$Q(h) = \delta(h^\theta - \hat{h}^\theta)Q(h^{(1)}, \dots, h^{(T)}).$$

- IID data: The training cases are independent, so

$$Q(h) = \delta(h^\theta - \hat{h}^\theta) \prod_{t=1}^T Q(h^{(t)}).$$

- Free energy:

$$F(Q, P) = -\log P(\hat{h}^\theta) + \sum_{t=1}^T \left(\int_{h^{(t)}} Q(h^{(t)}) \log \frac{Q(h^{(t)})}{P(h^{(t)}, v^{(t)} | \hat{h}^\theta)} \right).$$

The EM Algorithm

Initialization. Choose values for the parameters, \hat{h}^θ (randomly, or cleverly).

E Step. Minimize $F(Q, P)$ w.r.t. Q by setting

$$Q(h^{(t)}) \leftarrow P(h^{(t)} | v^{(t)}, \hat{h}^\theta),$$

for each training case, given the parameters \hat{h}^θ and the data $v^{(t)}$.

M Step. Minimize $F(Q, P)$ w.r.t. the model parameters \hat{h}^θ by solving

$$-\frac{\partial}{\partial \hat{h}^\theta} \log P(\hat{h}^\theta) - \sum_{t=1}^T \left(\int_{h^{(t)}} Q(h^{(t)}) \frac{\partial}{\partial \hat{h}^\theta} \log P(h^{(t)}, v^{(t)} | \hat{h}^\theta) \right) = 0. \quad (9)$$

For M parameters, this is a system of M equations. Often, the prior on the parameters is assumed to be uniform, $P(\hat{h}^\theta) = const$, in which case the first term in the above expression vanishes.

Repeat for a fixed number of iterations or until convergence.

Occlusion model: EM as an algorithm for minimizing the free energy

$$\begin{aligned}
 F(Q, P) &= \int_h Q(h) \log Q(h) - \int_h Q(h) \log P(h, v) \\
 &= \int_h Q(h) \log Q(h) - \int_{h^\theta} Q(h^\theta) \log P(h^\theta) - \\
 &\quad - \sum_{t=1}^T \int_{h^{(t)}, h^\theta} Q(h^{(t)}, h^\theta) \log P(h^{(t)}, v^{(t)} | h^\theta).
 \end{aligned}$$

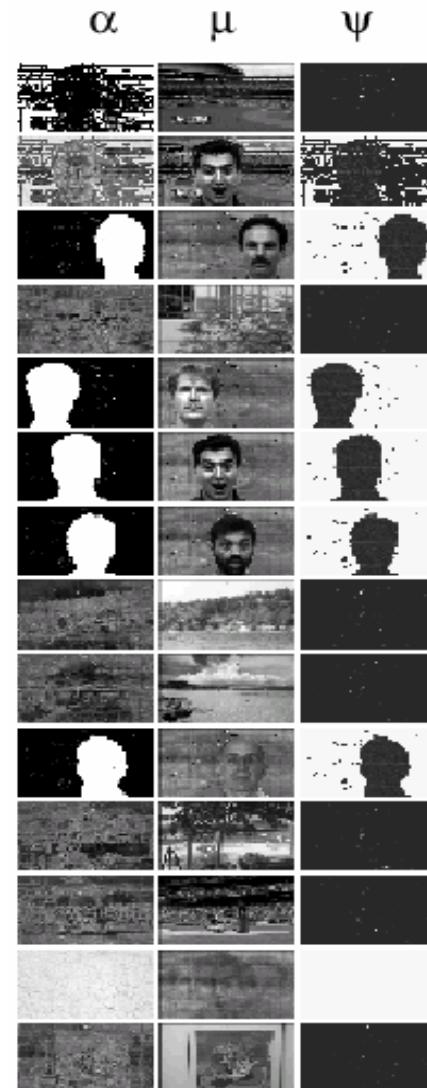
$$P \propto \prod_{t=1}^T (\pi_{f^{(t)}} \pi_{b^{(t)}} (\prod_{i=1}^K \alpha_{f^{(t)} i}^{m_i^{(t)}} (1 - \alpha_{f^{(t)} i})^{1-m_i^{(t)}} N(z_i^{(t)}; \mu_{f^{(t)} i}, \psi_{f^{(t)} i})^{m_i^{(t)}} N(z_i^{(t)}; \mu_{b^{(t)} i}, \psi_{b^{(t)} i})^{1-m_i^{(t)}})).$$

$$\begin{aligned}
 Q &= (\prod_k \delta(\pi_k - \hat{\pi}_k)) (\prod_{k,i} \delta(\mu_{ki} - \hat{\mu}_{ki})) (\prod_{k,i} \delta(\psi_{ki} - \hat{\psi}_{ki})) (\prod_{k,i} \delta(\alpha_{ki} - \hat{\alpha}_{ki})) \\
 &\quad \cdot Q(b, f) \prod_i Q(m_i | b, f).
 \end{aligned}$$

Occlusion model: EM as an algorithm for minimizing the free energy

E	$Q(m_i = 1 b, f) \leftarrow \frac{\alpha_{fi} N(z_i; \mu_{fi}, \psi_{fi})}{\alpha_{fi} N(z_i; \mu_{fi}, \psi_{fi}) + (1 - \alpha_{fi}) N(z_i; \mu_{bi}, \psi_{bi})},$ $Q(b, f) \leftarrow c \pi_b \pi_f \exp \left\{ - \sum_i (Q(m_i = 1 b, f) \left(\frac{(z_i - \mu_{fi})^2}{2\psi_{fi}} + \frac{\log 2\pi\psi_{fi}}{2} \right) + \right.$ $\left. (1 - Q(m_i = 1 b, f)) \left(\frac{(z_i - \mu_{bi})^2}{2\psi_{bi}} + \frac{\log 2\pi\psi_{bi}}{2} \right)) \right\},$	
M	$\pi_k \leftarrow (\sum_t Q(f^{(t)} = k) + \sum_t Q(b^{(t)} = k)) / (2T),$ $\alpha_{ki} \leftarrow \frac{\sum_t Q(m_i^{(t)} = 1, f^{(t)} = k)}{\sum_t Q(f^{(t)} = k)},$ $\mu_{ki} \leftarrow \frac{\sum_t (Q(m_i^{(t)} = 1, f^{(t)} = k) + Q(m_i^{(t)} = 0, b^{(t)} = k)) z_i^{(t)}}{\sum_t (Q(m_i^{(t)} = 1, f^{(t)} = k) + Q(m_i^{(t)} = 0, b^{(t)} = k))}.$ $\psi_{ki} \leftarrow \frac{\sum_t (Q(m_i^{(t)} = 1, f^{(t)} = k) + Q(m_i^{(t)} = 0, b^{(t)} = k)) (z_i^{(t)} - \mu_{ki})^2}{\sum_t (Q(m_i^{(t)} = 1, f^{(t)} = k) + Q(m_i^{(t)} = 0, b^{(t)} = k))}.$	$Q(b) \leftarrow \sum_f Q(b, f)$ $Q(f) \leftarrow \sum_b Q(b, f)$ $Q(m_i = 1, b) \leftarrow \sum_f Q(m_i = 1 b, f) Q(b, f)$ $Q(m_i = 1, f) \leftarrow \sum_b Q(m_i = 1 b, f) Q(b, f)$

Toy problem: Result of EM learning



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Generalizations of EM

- Update h^θ so as to only decrease F (not minimize F)
- Instead of updating Q using $Q(h^{(t)}) \leftarrow P(h^{(t)} | v^{(t)}, \hat{h}^\theta)$ update Q so as to only decrease F
- Use another inference technique for the Q -distribution over hidden variables...

Variational techniques

- Parameterize the Q-distribution: $Q(h; \phi)$
- Now, the *variational* free energy is

$$F(Q, P) = \int_h Q(h; \phi) \log \frac{Q(h; \phi)}{P(h, v)}.$$

- Computational task: Min F w.r.t ϕ
- Choose form of Q so math works out
- Example: Mean Field, $Q(h) = \prod_{i=1}^M Q(h_i),$

Variational inference

Initialization. Pick values for the variational parameters, ϕ (randomly, or cleverly).

Optimization Step. Decrease $F(Q, P)$ by adjusting the parameter vector ϕ , or a subset of ϕ .

Repeat for a fixed number of iterations or until convergence.

Variational EM

Initialization. Pick values for the variational parameters $\phi^{(1)}, \dots, \phi^{(T)}$ and the model parameters \hat{h}^θ (randomly, or cleverly).

Generalized E Step. Starting from the variational parameters from the previous iteration, modify $\phi^{(1)}, \dots, \phi^{(T)}$ so as to decrease F .

Generalized M Step. Starting from the model parameters from the previous iteration, modify \hat{h}^θ so as to decrease F .

Repeat for a fixed number of iterations or until convergence.

Occlusion model: Variational EM for minimizing the free energy

$$\begin{aligned}
 F(Q, P) &= \int_h Q(h) \log Q(h) - \int_h Q(h) \log P(h, v) \\
 &= \int_h Q(h) \log Q(h) - \int_{h^\theta} Q(h^\theta) \log P(h^\theta) - \\
 &\quad - \sum_{t=1}^T \int_{h^{(t)}, h^\theta} Q(h^{(t)}, h^\theta) \log P(h^{(t)}, v^{(t)} | h^\theta).
 \end{aligned}$$

$$P \propto \prod_{t=1}^T (\pi_{f^{(t)}} \pi_{b^{(t)}} (\prod_{i=1}^K \alpha_{f^{(t)} i}^{m_i^{(t)}} (1 - \alpha_{f^{(t)} i})^{1-m_i^{(t)}} N(z_i^{(t)}; \mu_{f^{(t)} i}, \psi_{f^{(t)} i})^{m_i^{(t)}} N(z_i^{(t)}; \mu_{b^{(t)} i}, \psi_{b^{(t)} i})^{1-m_i^{(t)}})).$$

$$\begin{aligned}
 Q &= (\prod_k \delta(\pi_k - \hat{\pi}_k)) (\prod_{k,i} \delta(\mu_{ki} - \hat{\mu}_{ki})) (\prod_{k,i} \delta(\psi_{ki} - \hat{\psi}_{ki})) (\prod_{k,i} \delta(\alpha_{ki} - \hat{\alpha}_{ki})) \\
 &\quad \cdot Q(b) Q(f) \prod_i Q(m_i). \qquad \text{VEM}
 \end{aligned}$$

Occlusion model: Variational EM for minimizing the free energy

$$\begin{aligned}
F = & \sum_b Q(b) \log \frac{Q(b)}{\pi_b} + \sum_f Q(f) \log \frac{Q(f)}{\pi_f} \\
& + \sum_i (q_i \log q_i + (1 - q_i) \log(1 - q_i)) - \sum_i (q_i (\sum_f Q(f) \log \alpha_{fi}) + (1 - q_i) (\sum_f Q(f) \log(1 - \alpha_{fi}))) \\
& + \sum_i \sum_f Q(f) q_i \left(\frac{(z_i - \mu_{fi})^2}{2\psi_{fi}} + \frac{\log 2\pi\psi_{fi}}{2} \right) + \sum_i \sum_b Q(b) (1 - q_i) \left(\frac{(z_i - \mu_{bi})^2}{2\psi_{bi}} + \frac{\log 2\pi\psi_{bi}}{2} \right).
\end{aligned}$$

$$P \propto \prod_{t=1}^T (\pi_{f^{(t)}} \pi_{b^{(t)}} (\prod_{i=1}^K \alpha_{f^{(t)}i}^{m_i^{(t)}} (1 - \alpha_{f^{(t)}i})^{1-m_i^{(t)}} N(z_i^{(t)}; \mu_{f^{(t)}i}, \psi_{f^{(t)}i})^{m_i^{(t)}} N(z_i^{(t)}; \mu_{b^{(t)}i}, \psi_{b^{(t)}i})^{1-m_i^{(t)}})).$$

$$\begin{aligned}
Q = & (\prod_k \delta(\pi_k - \hat{\pi}_k)) (\prod_{k,i} \delta(\mu_{ki} - \hat{\mu}_{ki})) (\prod_{k,i} \delta(\psi_{ki} - \hat{\psi}_{ki})) (\prod_{k,i} \delta(\alpha_{ki} - \hat{\alpha}_{ki})) \\
& \cdot Q(b) Q(f) \prod_i Q(m_i). \quad \text{VEM}
\end{aligned}$$

Occlusion model: Comparison of exact EM with Variational EM

Class	v_f	v_b	α	μ	Ψ	v_f	v_b	α	μ	Ψ
1	0.04	0.11				0.06	0.07			
2	0	0.04				0.07	0.12			
3	0.20	0				0.07	0.04			
4	0	0.14				0.07	0.06			
5	0.19	0				0.07	0.15			
6	0.17	0				0.09	0.07			
7	0.19	0				0.10	0.03			
8	0	0.13				0.03	0.08			
9	0	0.13				0.09	0.06			
10	0.21	0				0.02	0.03			
11	0	0.12				0.10	0.04			
12	0	0.17				0.04	0.06			
13	0	0				0.07	0.15			
14	0	0.16				0.12	0.04			

```
graph TD; A[Exact EM] --> B[Variational EM]; A --> C["Foreground and background frequencies"]
```

Structured variational techniques

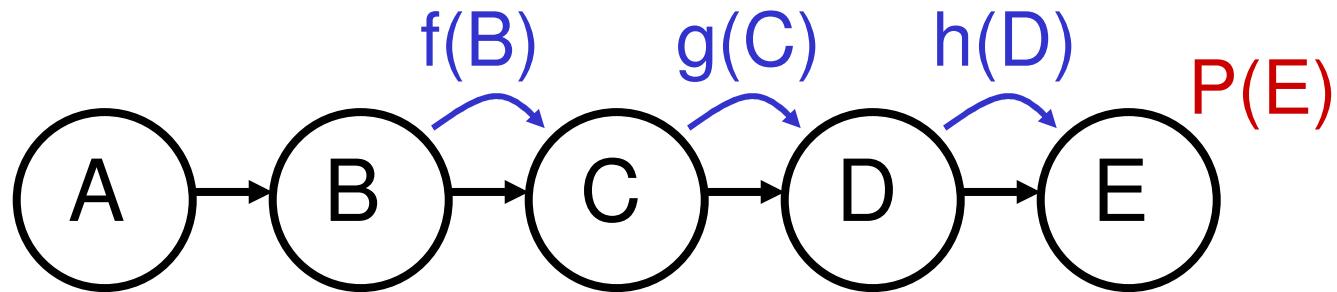
- We can also describe Q using a parameterized graphical model
- Choose the structure and form of Q so that

$$F(Q, P) = \int_h Q(h; \phi) \log \frac{Q(h; \phi)}{P(h, v)}.$$

is tractable

- Structured variational technique for toy problem: See tutorial paper

The sum-product algorithm (belief propagation)



$$P(A, B, C, D, E) = P(E|D)P(D|C)P(C|B)P(B|A)P(A)$$

$$P(E) = \sum_D \sum_C \sum_B \sum_A P(E|D)P(D|C)P(C|B)P(B|A)P(A)$$

$$= \sum_D P(E|D) [\sum_C P(D|C) [\sum_B P(C|B) [\sum_A P(B|A)P(A)]]]$$

$$\begin{array}{c} f(B) \\ g(C) \\ h(D) \end{array}$$

SP Algorithm as Free Energy Minimization

For a graphical model with potentials, $\Psi_j(x_{Cj})$ on cliques x_{Cj} ,

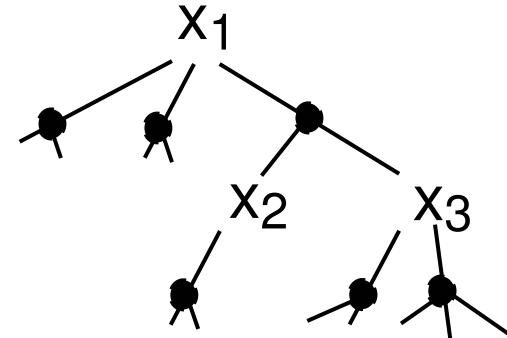
$$F = -\sum_j \sum_{x_{Cj}} Q(x_{Cj}) \log[\Psi_j(x_{Cj})] + \sum_x Q(x) \log[Q(x)]$$

- For a general Q -distribution, if $Q(x_{Cj})$ are known, the 1st term is easy to compute
- Problem: 2nd term is generally intractable
- Idea: Represent $Q(x)$ by $Q(x_j)$, $\forall j$, and $Q(x_{Cj})$, $\forall i$, and approximate the 2nd term

Bethe approximation

- For a tree

$$Q(x) = \frac{\prod_i Q(x_{C_i})}{\prod_j Q(x_j)^{d_j - 1}}$$



- d_j = degree of x_j
- Use this expression for the entropy, even when the graph is not a tree
- Note: For a tree, the minimizer of F gives $Q(x) = P(x)$: Exact inference

Solving for Q

$$F = -\sum_i \sum_{x_{C_i}} Q(x_{C_i}) \log [\Psi_i(x_{C_i})]$$

$$+ \sum_i \sum_{x_{C_i}} Q(x_{C_i}) \log [Q(x_{C_i})] - \sum_j (d_j - 1) \sum_{x_j} Q(x_j) \log [Q(x_j)]$$

Solve $\partial D / \partial Q(x_{C_i}) = 0$ and $\partial D / \partial Q(x_j) = 0$,
subject to the constraints

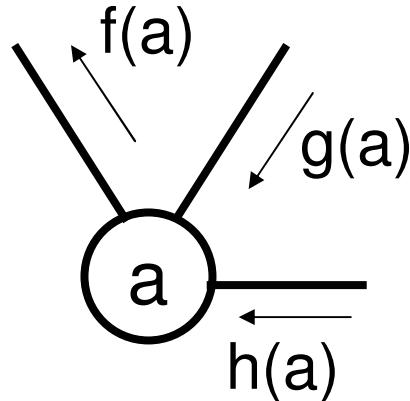
- $\sum_{x_j} Q(x_j) = 1$
- $\sum_{x_{C_i}} Q(x_{C_i}) = 1$
- For $j \in C_i$, $\sum_{x_{C_i} \setminus j} Q(x_{C_i}) = Q(x_j)$

Result (Yedidia et al 2001): Sum-product algorithm

The sum-product algorithm

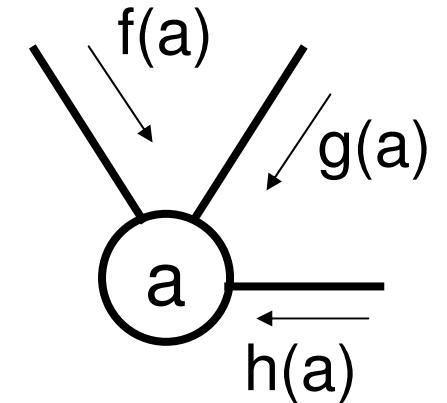
Each message is a function of its neighboring variable

Out of variable



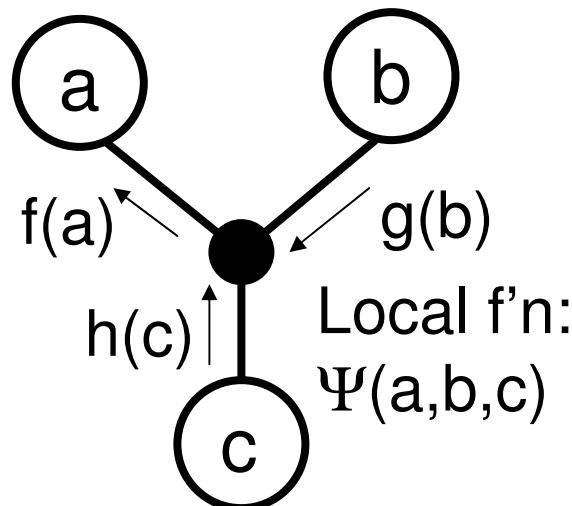
$$f(a) = g(a)h(a)$$

Fusion



$$P(a) \approx f(a)g(a)h(a)$$

Out of function



$$f(a) = \sum_b \sum_c \Psi(a,b,c) g(b) h(c)$$

Occlusion model: The sum-product algorithm

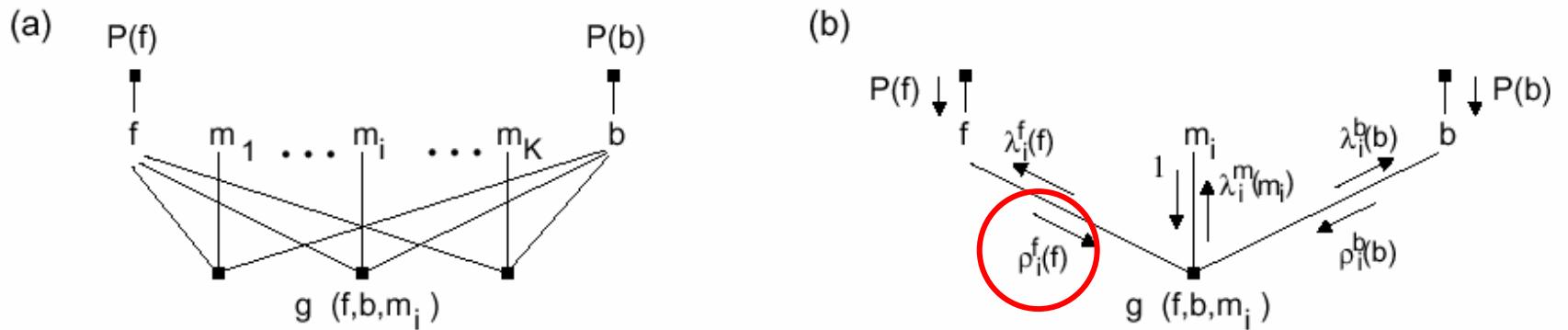


$$\begin{aligned}
 g_i(f, b, m_i) &= P(z_i | m_i, f, b)P(m_i | f) = \\
 &N(z_i; \mu_{fi}, \psi_{fi})^{m_i} N(z_i; \mu_{bi}, \psi_{bi})^{1-m_i} \alpha_{fi}^{m_i} (1 - \alpha_{fi})^{1-m_i}.
 \end{aligned}$$

$$\lambda_i^f(f) \leftarrow \alpha_{fi} N(z_i; \mu_{fi}, \psi_{fi}) + (1 - \alpha_{fi}) \sum_b N(z_i; \mu_{bi}, \psi_{bi}) \rho_i^b(b).$$

$$\lambda_i^f(f) \leftarrow \lambda_i^f(f) / (\sum_f \lambda_i^f(f))$$

Occlusion model: The sum-product algorithm

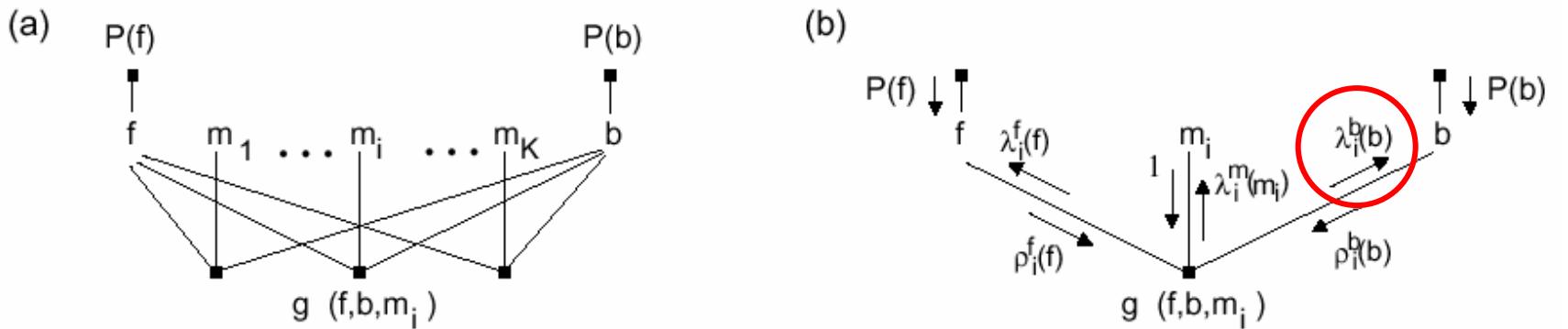


$$\begin{aligned}
 g_i(f, b, m_i) &= P(z_i | m_i, f, b) P(m_i | f) = \\
 &N(z_i; \mu_{fi}, \psi_{fi})^{m_i} N(z_i; \mu_{bi}, \psi_{bi})^{1-m_i} \alpha_{fi}^{m_i} (1 - \alpha_{fi})^{1-m_i}.
 \end{aligned}$$

$$\rho_i^f(f) \leftarrow P(f) \prod_{j \neq i} \lambda_i^f(f),$$

$$\rho_i^f(f) \leftarrow \rho_i^f(f) / (\sum_f \rho_i^f(f))$$

Occlusion model: The sum-product algorithm

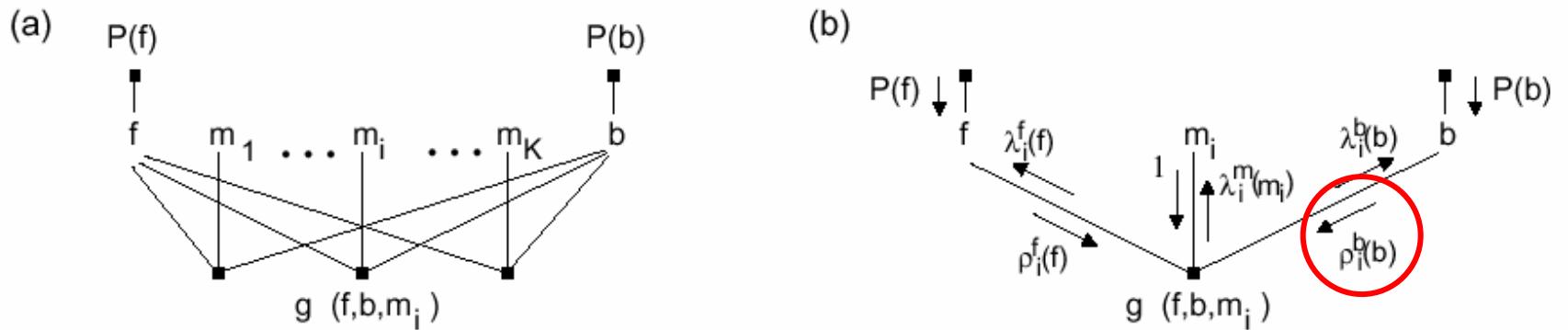


$$\begin{aligned}
 g_i(f, b, m_i) &= P(z_i | m_i, f, b) P(m_i | f) = \\
 &N(z_i; \mu_{fi}, \psi_{fi})^{m_i} N(z_i; \mu_{bi}, \psi_{bi})^{1-m_i} \alpha_{fi}^{m_i} (1 - \alpha_{fi})^{1-m_i}.
 \end{aligned}$$

$$\lambda_i^b(b) \leftarrow \sum_f \sum_{m_i} g_i(f, b, m_i) \cdot 1 \cdot \rho_i^f(f)$$

$$\lambda_i^b(b) \leftarrow \lambda_i^b(b) / (\sum_b \lambda_i^b(b))$$

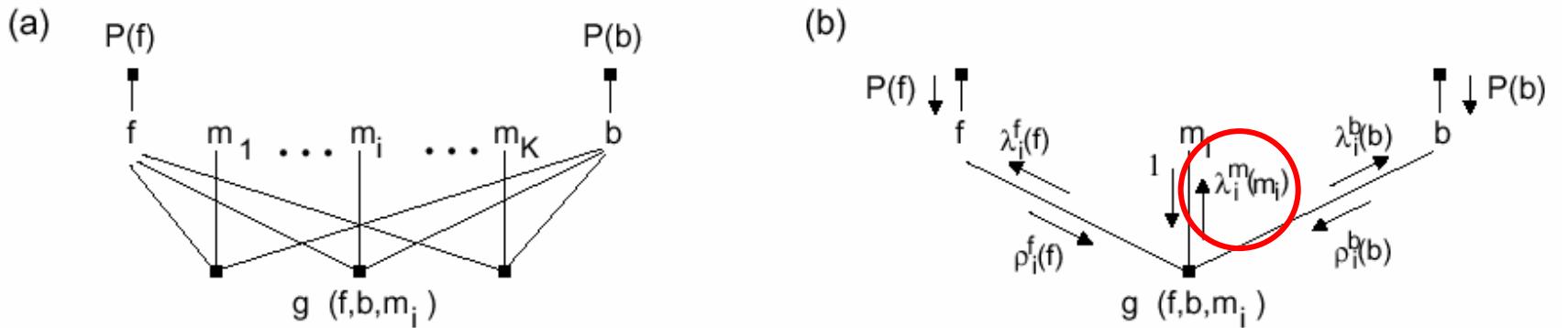
Occlusion model: The sum-product algorithm



$$\begin{aligned}
 g_i(f, b, m_i) &= P(z_i | m_i, f, b) P(m_i | f) = \\
 &N(z_i; \mu_{fi}, \psi_{fi})^{m_i} N(z_i; \mu_{bi}, \psi_{bi})^{1-m_i} \alpha_{fi}^{m_i} (1 - \alpha_{fi})^{1-m_i}.
 \end{aligned}$$

$$\begin{aligned}
 \rho_i^b(b) &\leftarrow P(b) \prod_{j \neq i} \lambda_i^b(b), \\
 \rho_i^b(b) &\leftarrow \rho_i^b(b) / (\sum_b \rho_i^b(b))
 \end{aligned}$$

Occlusion model: The sum-product algorithm



$$g_i(f, b, m_i) = P(z_i | m_i, f, b)P(m_i | f) = \\ N(z_i; \mu_{fi}, \psi_{fi})^{m_i} N(z_i; \mu_{bi}, \psi_{bi})^{1-m_i} \alpha_{fi}^{m_i} (1 - \alpha_{fi})^{1-m_i}.$$

$$\lambda_i^m(m_i) \leftarrow \sum_f \sum_b g_i(f, b, m_i) \cdot \rho_i^f(f) \cdot \rho_i^b(b) :$$

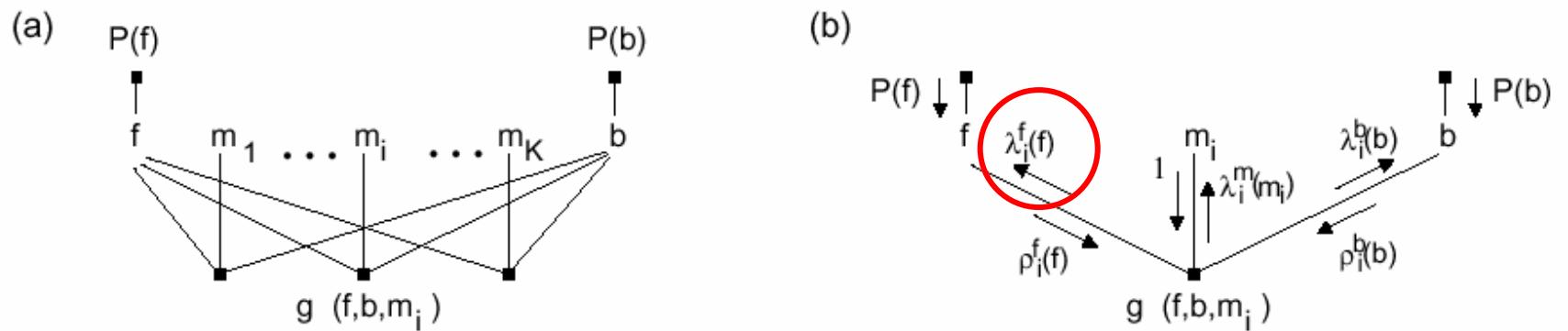
$$\lambda_i^m(1) \leftarrow \sum_f N(z_i; \mu_{fi}, \psi_{fi}) \alpha_{fi} \rho_i^f(f),$$

$$\lambda_i^m(0) \leftarrow (\sum_b N(z_i; \mu_{bi}, \psi_{bi}) \rho_i^b(b)) (\sum_f (1 - \alpha_{fi}) \rho_i^f(f)).$$

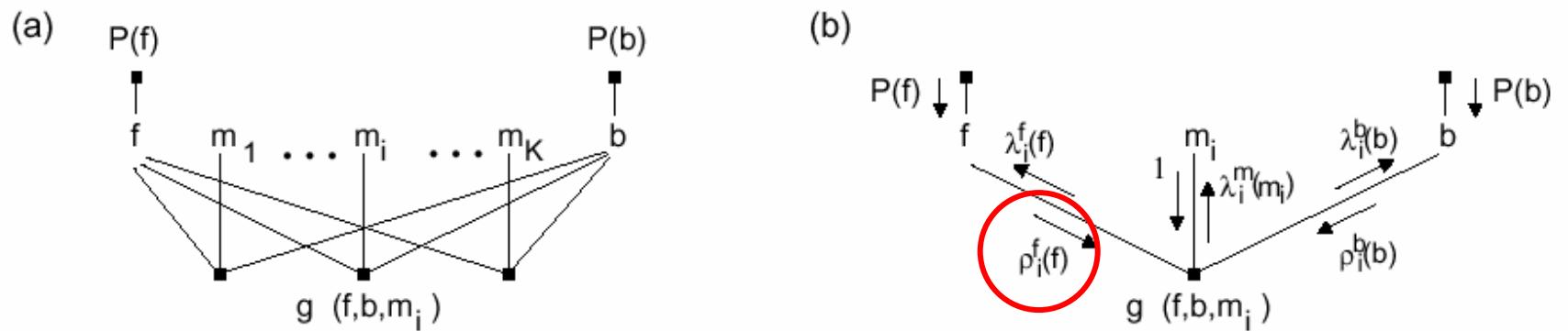
$$\lambda_i^m(m_i) \leftarrow \lambda_i^m(m_i) / (\lambda_i^m(0) + \lambda_i^m(1))$$

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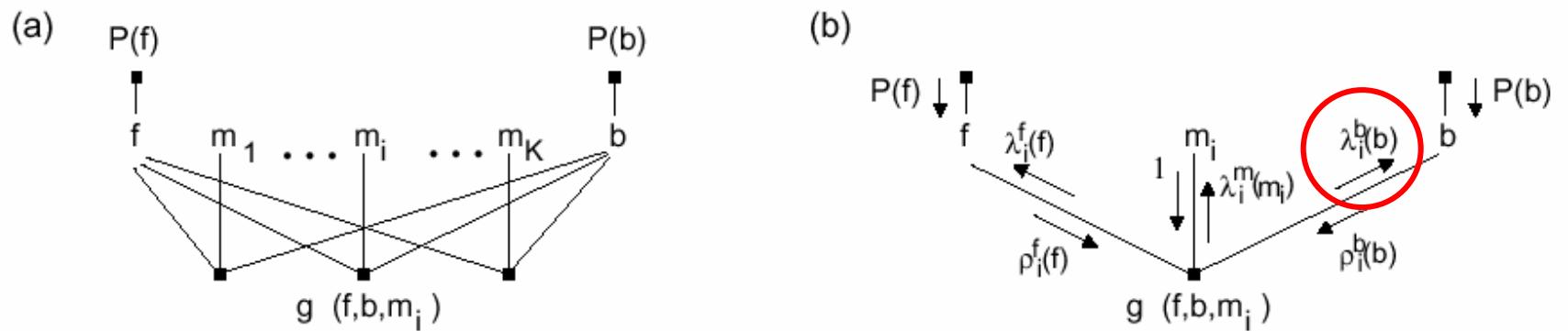
Occlusion model: The sum-product algorithm



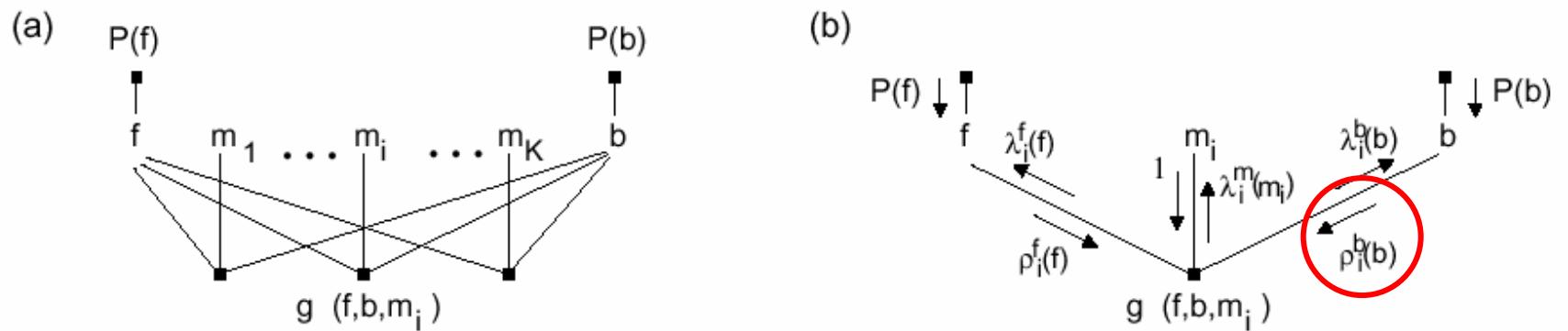
Occlusion model: The sum-product algorithm



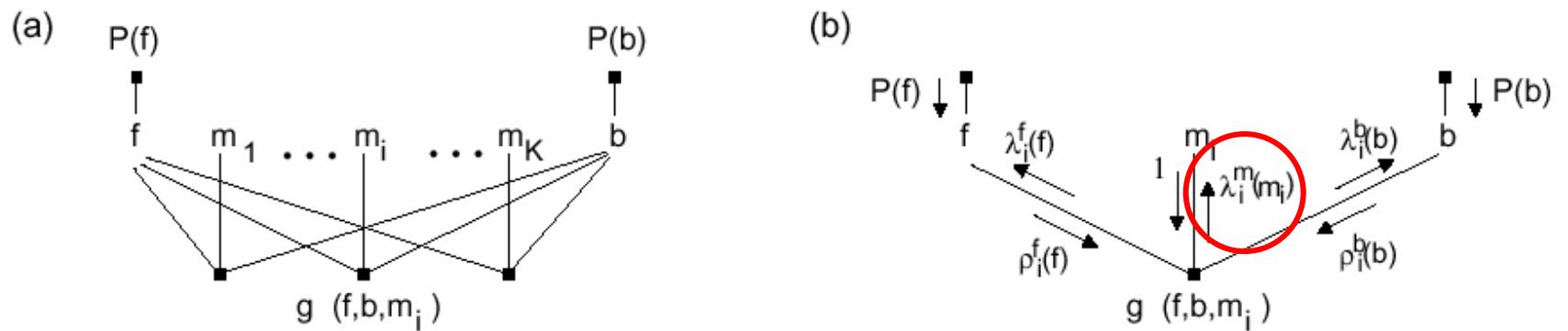
Occlusion model: The sum-product algorithm



Occlusion model: The sum-product algorithm



Occlusion model: The sum-product algorithm



Gibbs sampling

- The posterior $P(h_1, h_2, \dots, h_K | v)$ is not tractable, but often, the conditionals, $P(h_i | h \setminus h_i, v)$, can be sampled from
- Gibbs sampling:

Initialization. Pick values for all hidden variables (randomly, or cleverly).

Sampling Step. Choose a variable h_i at random or in order, and then sample it from $P(h_i | h \setminus h_i)$.

Repeat for a fixed number of iterations or until convergence.

Gibbs sampling as free energy minimization

- Imagine running an ensemble of Gibbs chains in parallel
- Let $Q^n(h)$ describe the distribution of the h 's at step n of the sampling procedure
- Suppose at step n , we sample h_i in every chain:
$$Q^{n+1}(h) = Q^n(h \setminus h_i)P(h_i|h \setminus h_i, v)$$

- Substituting these into the expression for F , we find that $F^{n+1} \leq F^n$

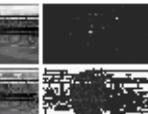
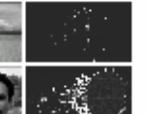
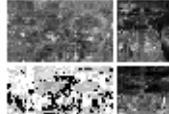
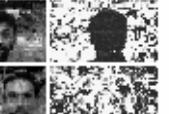
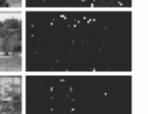
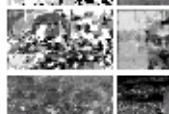
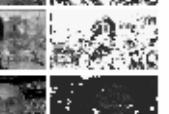
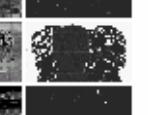
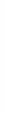
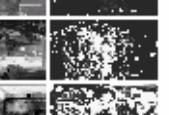
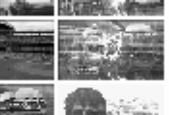
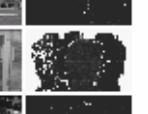
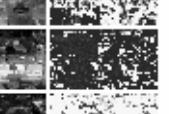
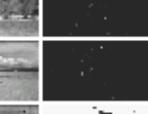
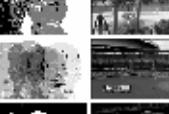
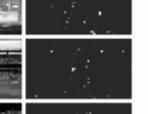
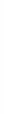
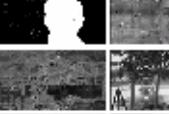
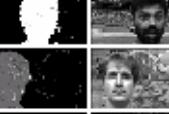
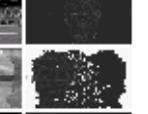
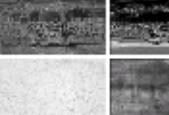
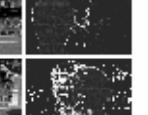
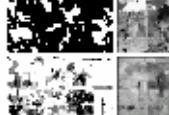
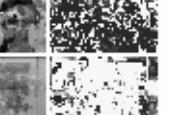
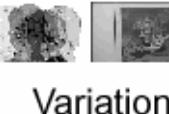
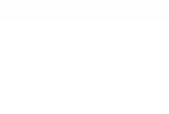
Discussion of Algorithms

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Comparison of algorithms for occlusion model

Method	Update for mask variables	Complexity
Exact inference (used in EM)	$\frac{Q(m_i=1 b,f)}{Q(m_i=0 b,f)} \leftarrow \frac{\alpha_{fi}\mathcal{N}(z_i;\mu_{fi},\psi_{fi})}{(1-\alpha_{fi})\mathcal{N}(z_i;\mu_{bi},\psi_{bi})}$	$J^2 K$
Iterative conditional modes	$m_i \leftarrow \begin{cases} 1, & \text{if } \frac{\alpha_{fi}\mathcal{N}(z_i;\mu_{fi},\psi_{fi})}{(1-\alpha_{fi})\mathcal{N}(z_i;\mu_{bi},\psi_{bi})} > 1 \\ 0, & \text{otherwise} \end{cases}$	K
Gibbs sampling	$m_i \leftarrow \text{sample}_{m_i} \left\{ \begin{array}{ll} \alpha_{fi}\mathcal{N}(z_i;\mu_{fi},\psi_{fi}) & \text{if } m_i = 1 \\ (1 - \alpha_{fi})\mathcal{N}(z_i;\mu_{bi},\psi_{bi}) & \text{if } m_i = 0 \end{array} \right\}$	K
Fully-factorized variational	$\frac{Q(m_i=1)}{Q(m_i=0)} \leftarrow \frac{\prod_f (\alpha_{fi}\mathcal{N}(z_i;\mu_{fi},\psi_{fi}))^{Q(f)}}{(\prod_f (1-\alpha_{fi}))^{Q(f)} (\prod_b \mathcal{N}(z_i;\mu_{bi},\psi_{bi}))^{Q(b)})}$	JK
Structured variational	$\frac{Q(m_i=1 f)}{Q(m_i=0 f)} \leftarrow \frac{\alpha_{fi}\mathcal{N}(z_i;\mu_{fi},\psi_{fi})}{(1-\alpha_{fi}) \prod_b \mathcal{N}(z_i;\mu_{bi},\psi_{bi})^{Q(b)}}$	JK
Sum-product algorithm	$\frac{Q(m_i=1)}{Q(m_i=0)} \leftarrow \frac{\sum_f \rho_i^f(f) \alpha_{fi}\mathcal{N}(z_i;\mu_{fi},\psi_{fi})}{(\sum_f \rho_i^f(f)(1-\alpha_{fi}))(\sum_b \rho_i^b(b)\mathcal{N}(z_i;\mu_{bi},\psi_{bi}))}$	JK

Experimental results for occlusion model

Class	v_f	v_b	α	μ	Ψ	v_f	v_b	α	μ	Ψ	α	μ	Ψ	α	μ	Ψ
1	0.04	0.11				0.06	0.07									
2	0	0.04				0.07	0.12									
3	0.20	0				0.07	0.04									
4	0	0.14				0.07	0.06									
5	0.19	0				0.07	0.15									
6	0.17	0				0.09	0.07									
7	0.19	0				0.10	0.03									
8	0	0.13				0.03	0.08									
9	0	0.13				0.09	0.06									
10	0.21	0				0.02	0.03									
11	0	0.12				0.10	0.04									
12	0	0.17				0.04	0.06									
13	0	0				0.07	0.15									
14	0	0.16				0.12	0.04									

Exact EM

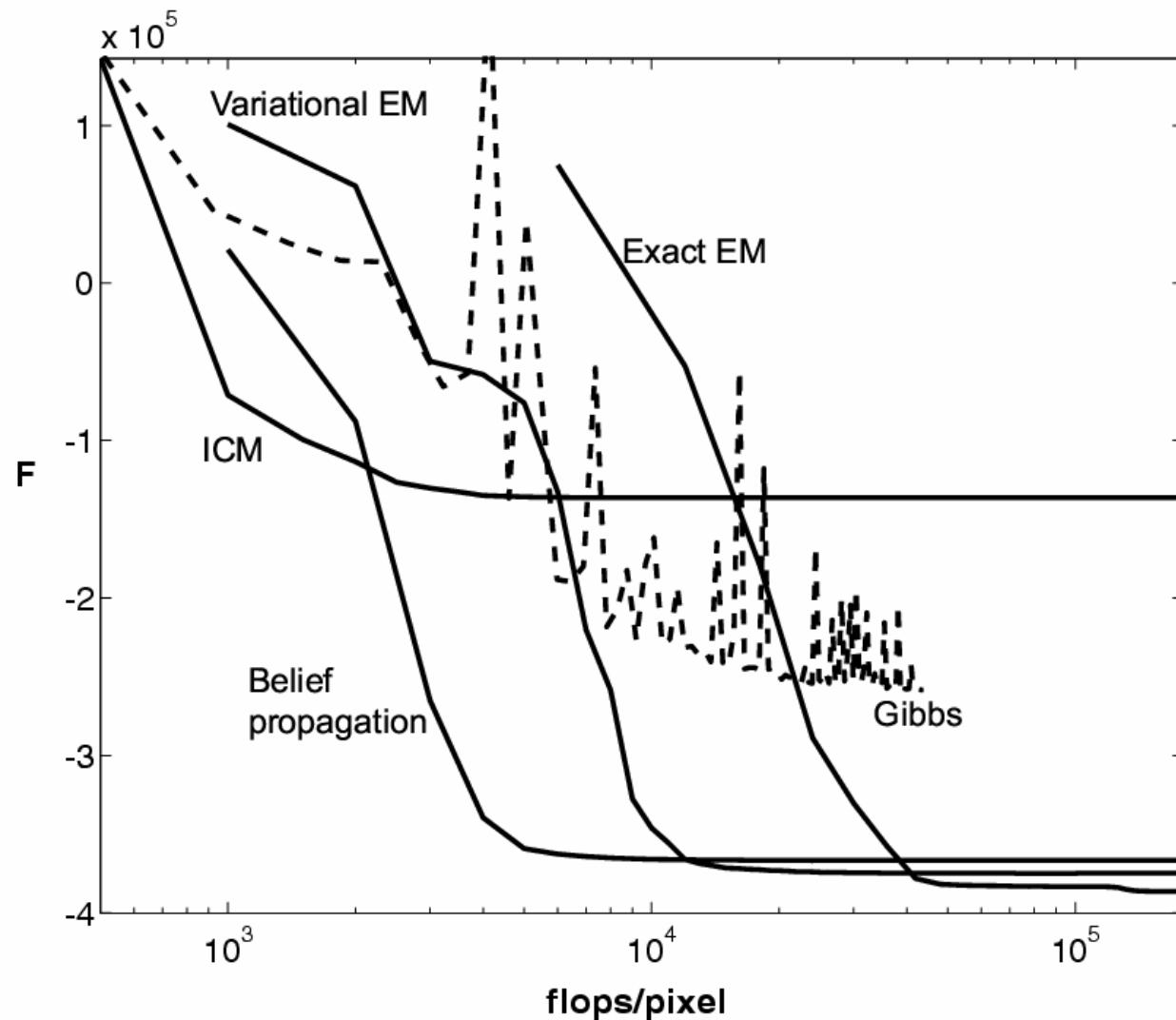
Variational EM

ICM

Belief propagation

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Speed of convergence



Recall: From ICM to Gibbs sampling

Sample

- For $t = 1, \dots, T$

$$\{ f^{(t)} \leftarrow \operatorname{argmax}_{f^{(t)}} [\pi_{f^{(t)}} \prod_{i:m_i^{(t)}=1} \mathcal{N}(z_i^{(t)}; \mu_{f^{(t)}i}, \psi_{f^{(t)}i})]$$

$$\{ b^{(t)} \leftarrow \operatorname{argmax}_{b^{(t)}} [\pi_{b^{(t)}} \prod_{i:m_i^{(t)}=0} \mathcal{N}(z_i^{(t)}; \mu_{b^{(t)}i}, \psi_{b^{(t)}i})]$$

$$\{ \text{For } i = 1, \dots, K: m_i^{(t)} \leftarrow \begin{cases} 1 & \text{if } \alpha_{f^{(t)}i} \mathcal{N}(z_i^{(t)}; \mu_{f^{(t)}i}, \psi_{f^{(t)}i}) > (1 - \alpha_{f^{(t)}i}) \mathcal{N}(z_i^{(t)}; \mu_{b^{(t)}i}, \psi_{b^{(t)}i}) \\ 0 & \text{otherwise} \end{cases}$$

- For $j = 1, \dots, J$

$$\{ \pi_j \leftarrow (\sum_{t=1}^T [f^{(t)} = j] + \sum_{t=1}^T [b^{(t)} = j]) / 2T$$

- For $j = 1, \dots, J$, for $i = 1, \dots, K$

$$\{ \alpha_{ji} \leftarrow (\sum_{t=1}^T [f^{(t)} = j] m_i^{(t)}) / (\sum_{t=1}^T [f^{(t)} = j])$$

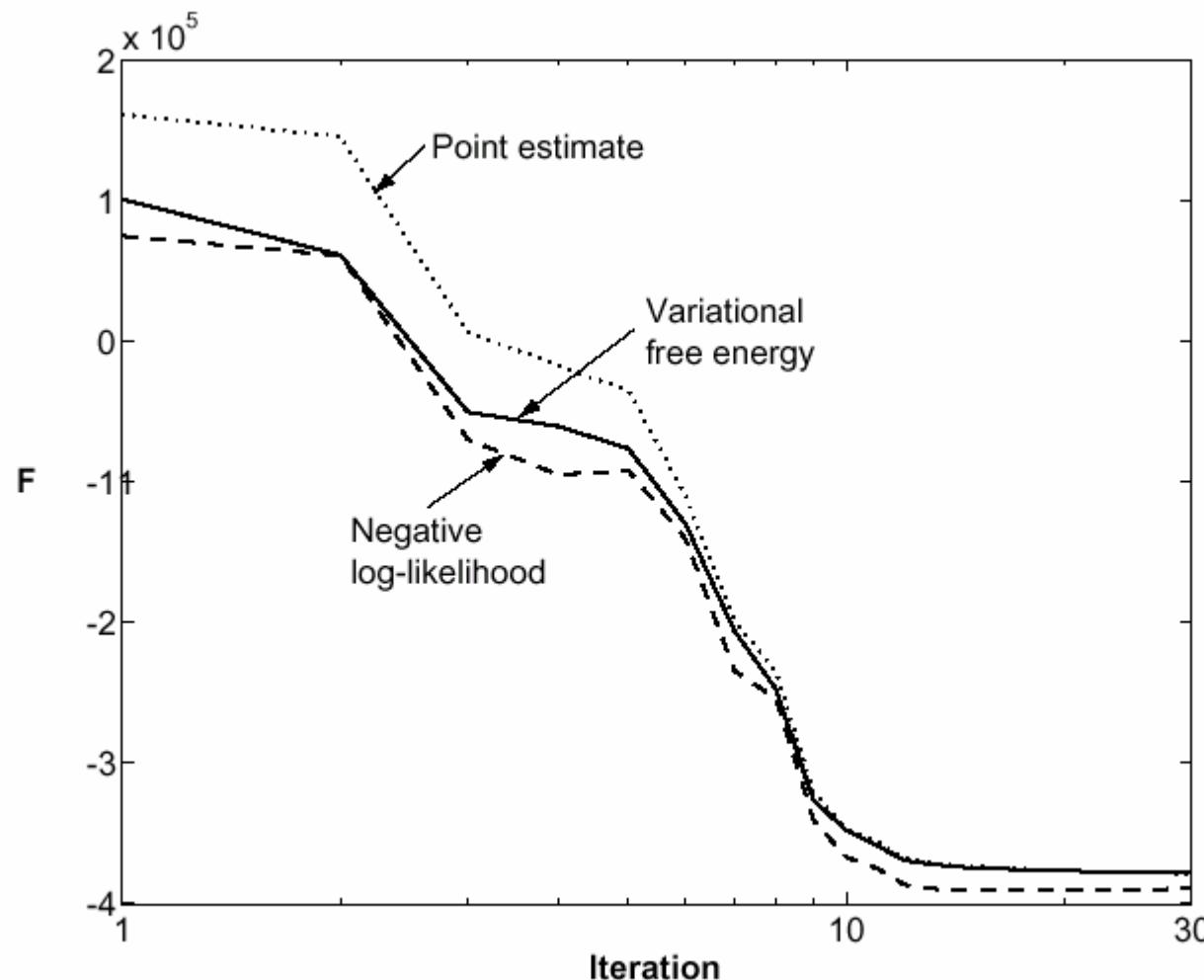
$$\{ \mu_{ji} \leftarrow (\sum_{t=1}^T [f^{(t)} = j \text{ or } b^{(t)} = j] z_i^{(t)}) / (\sum_{t=1}^T [f^{(t)} = j \text{ or } b^{(t)} = j])$$

$$\{ \psi_{ji} \leftarrow (\sum_{t=1}^T [f^{(t)} = j \text{ or } b^{(t)} = j] (z_i^{(t)} - \mu_{ji})^2) / (\sum_{t=1}^T [f^{(t)} = j \text{ or } b^{(t)} = j])$$

Here, the Iverson notation is used where [True] = 1 and [False] = 0.

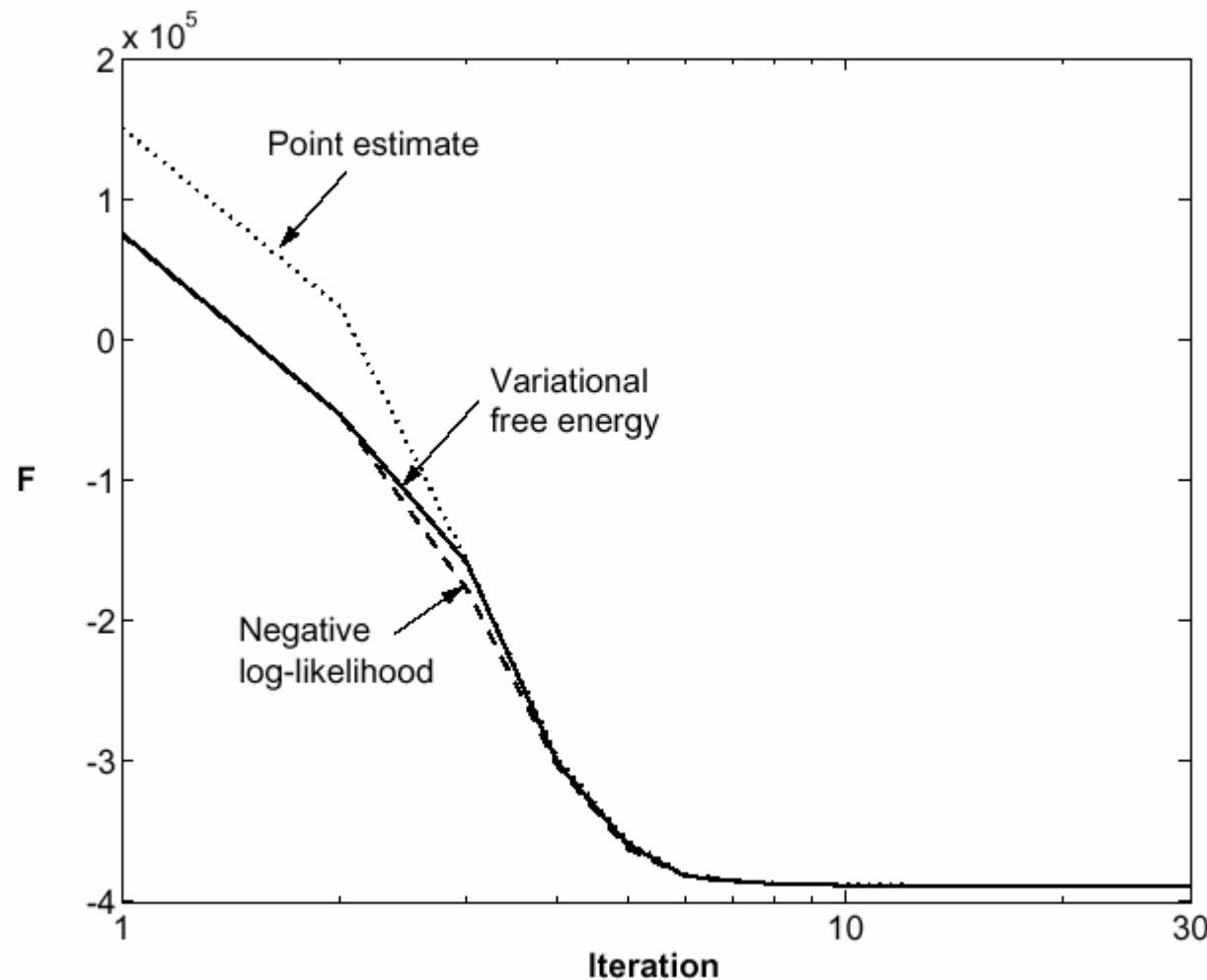
How tight are the bounds?

Various bounds during variational learning



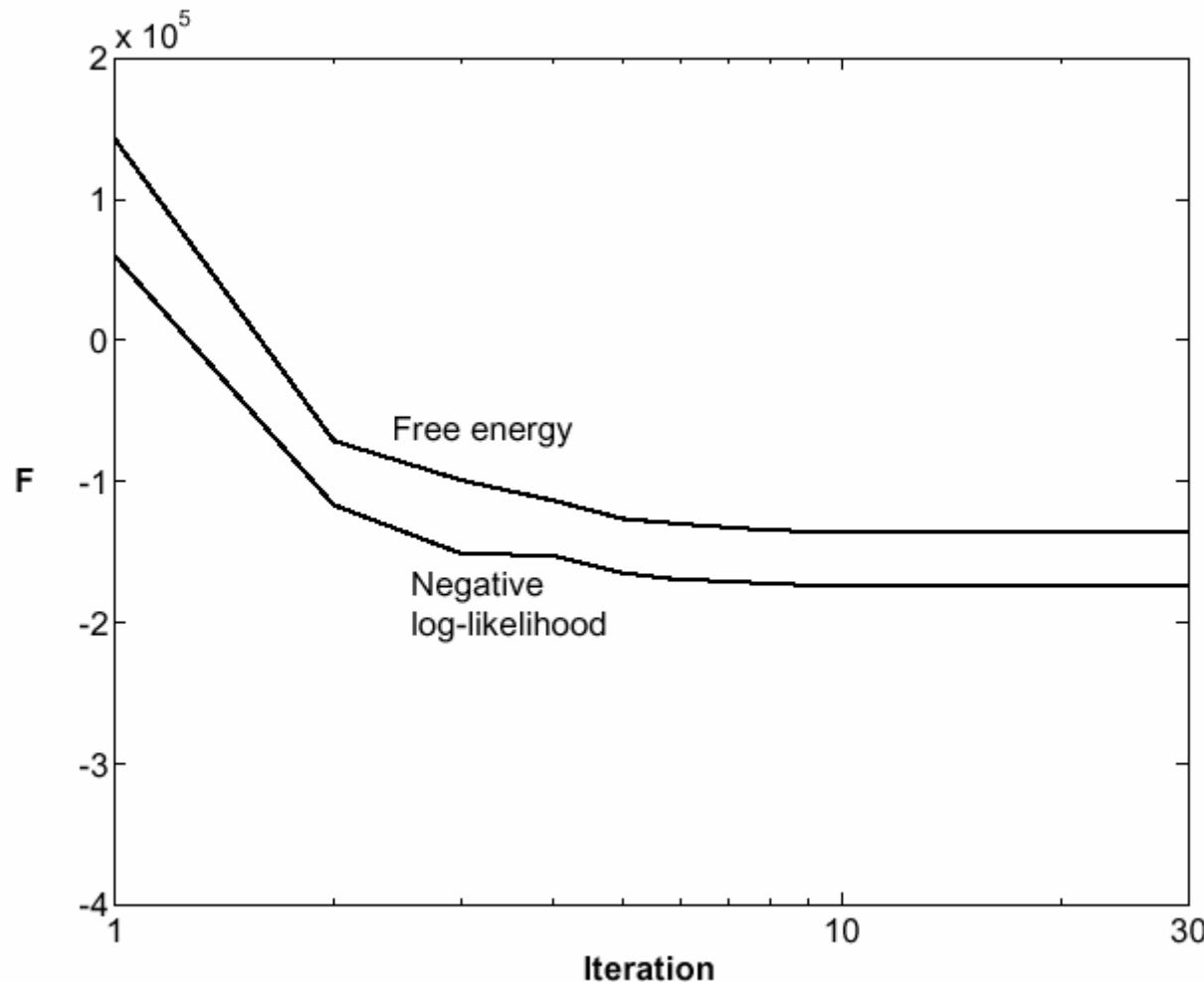
How tight are the bounds?

Various bounds during EM learning

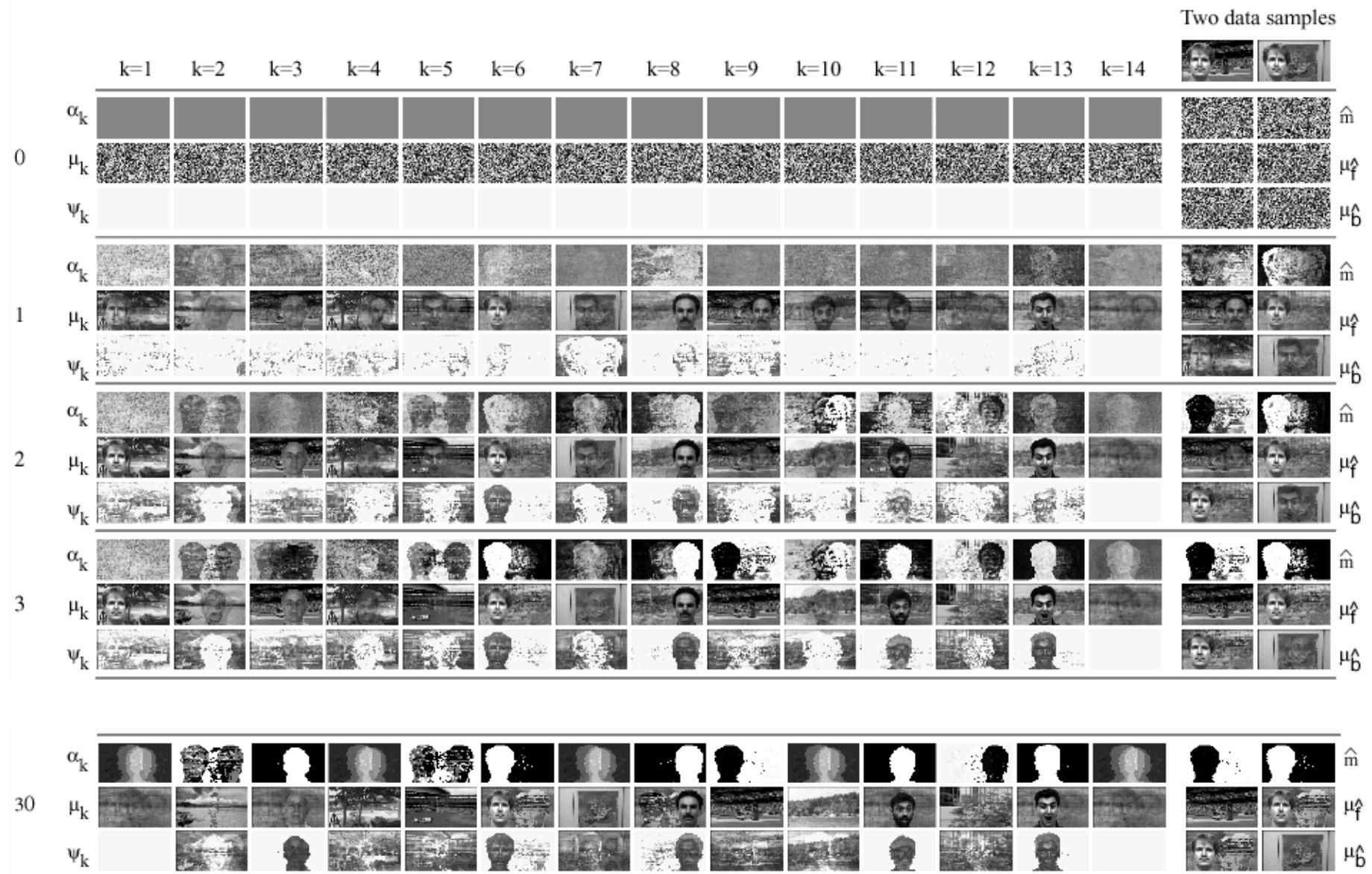


How tight are the bounds?

Various bounds during ICM learning



Iterative model optimization (sum-product algorithm)



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Improving approximate methods with additional EM iterations



Wrap-up

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The Art

- Representation is critical
- Structure versus forms of probability functions
- What computation should the graph be used for (eg, recursive updates or coordinated optimization)?
- Which is better: Exact inference in inaccurate models or approximate inference in accurate models?
- ...

Application: Cardboard cut-out scene analysis

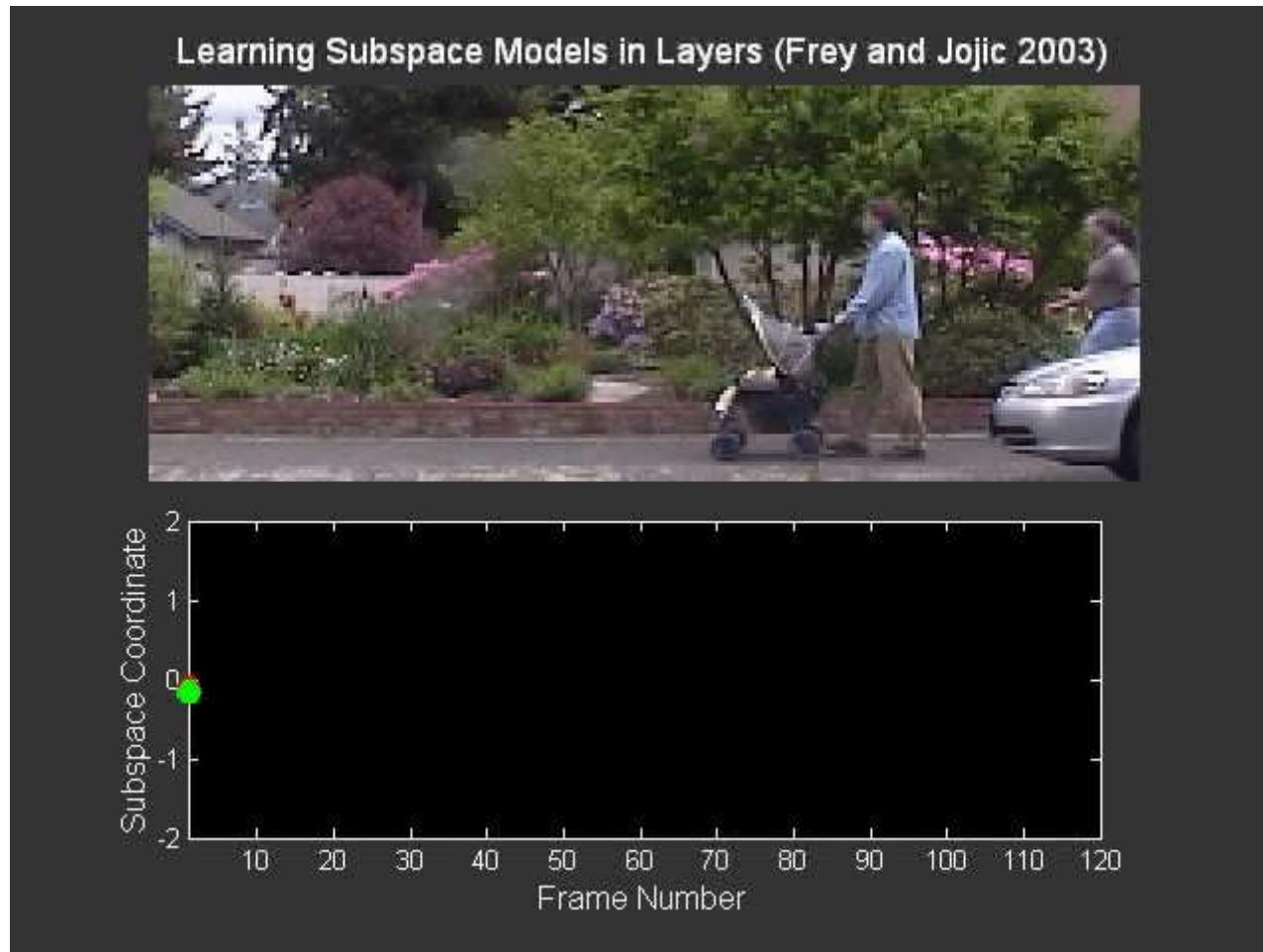
Jojic and Frey, CVPR 2001



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Application: Subspace models of occluding objects in 3-D scenes

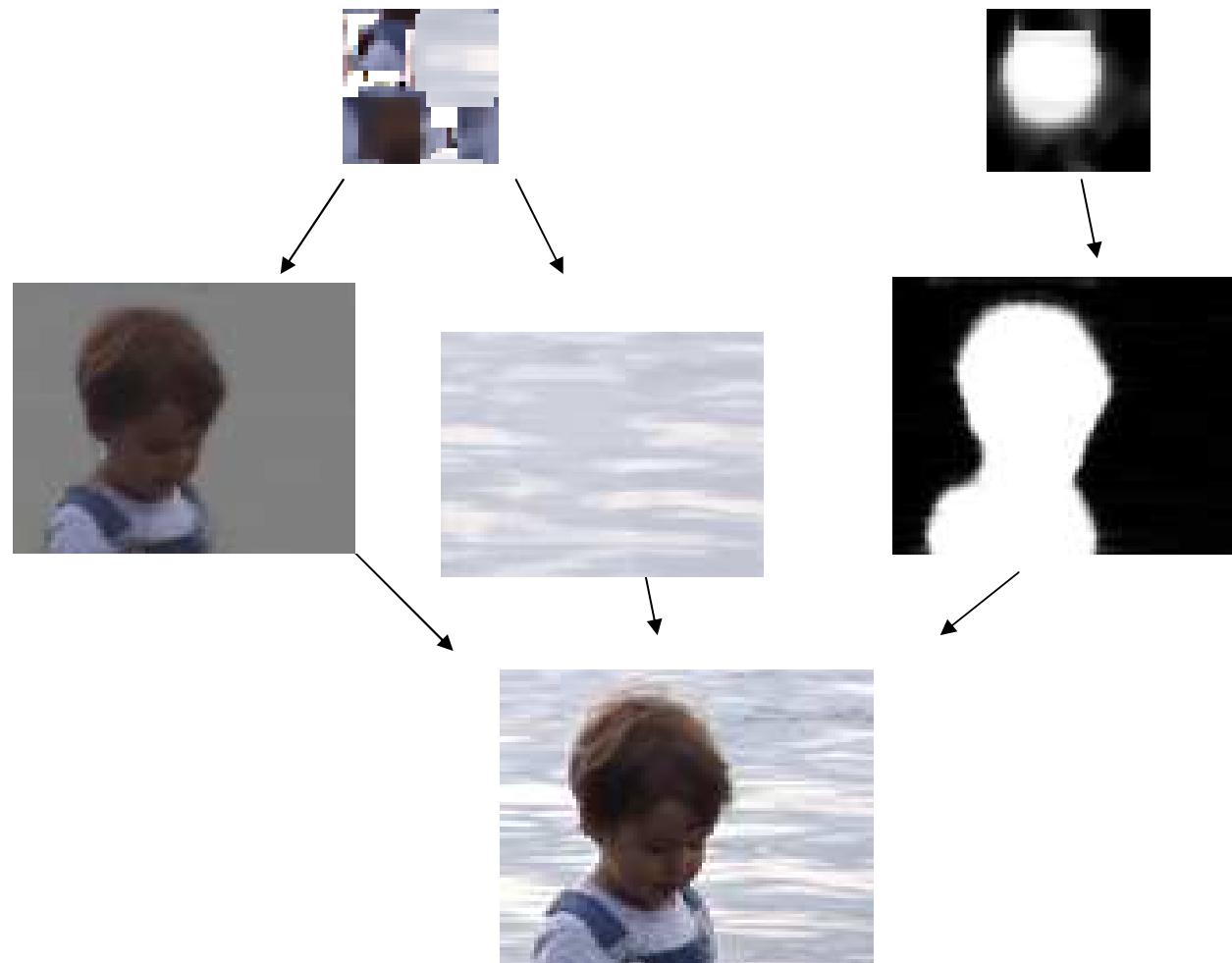
Frey, Jojic and Kannan 2003



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Application: Scene interpretation from single images

Jojic, Frey and Kannan 2003



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- Those are the basics
- Go forth, model, perform approximate inference, and have fun!