# Part 3: Probabilistic Inference in Graphical Models

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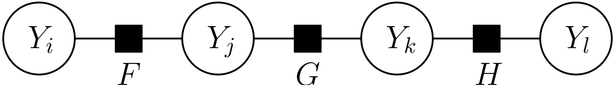
Microsoft Research
IST AUSTRIA Institute of Science and Technology

# Belief Propagation

- “Message-passing” algorithm
- Exact and optimal for tree-structured graphs
- Approximate for cyclic graphs

# Example: Inference on Chains

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Z &= \sum_{y \in \mathcal{Y}} \exp(-E(y)) \\
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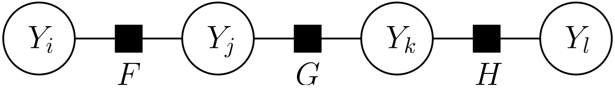


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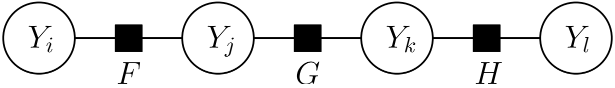


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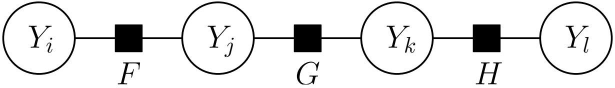


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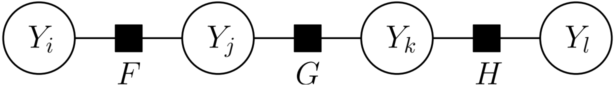


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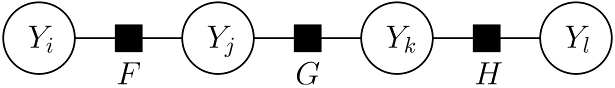


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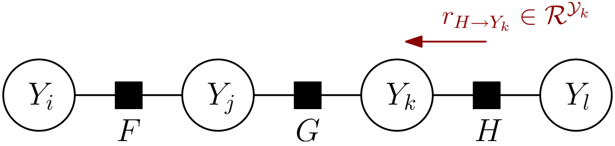


$$Z = \sum_{y_i\in\mathcal{Y}_i}\sum_{y_j\in\mathcal{Y}_j}\exp(-E_F(y_i,y_j))\sum_{y_k\in\mathcal{Y}_k}\exp(-E_G(y_j,y_k))\underbrace{\sum_{y_l\in\mathcal{Y}_l}\exp(-E_H(y_k,y_l))}_{r_{H\to Y_k}(y_k)}$$

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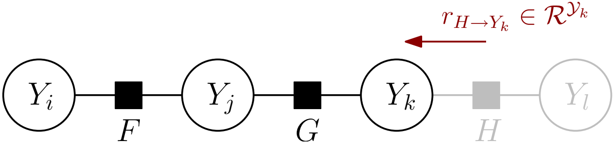


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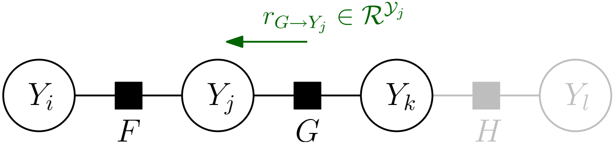


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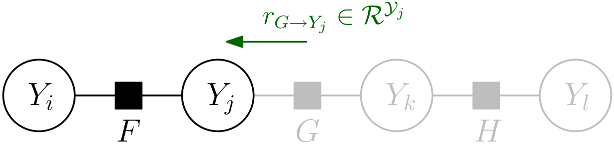


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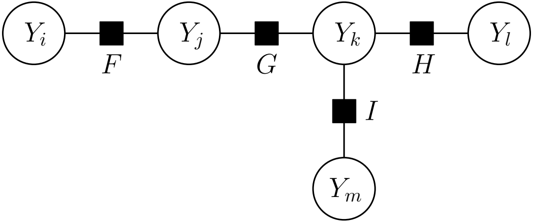
# Example: Inference on Trees

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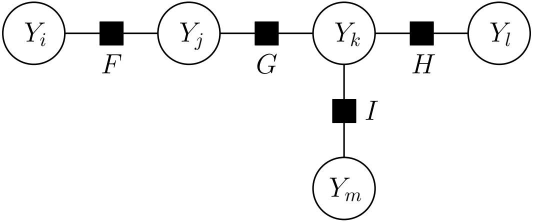


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$$\left( \underbrace{\left( \sum_{y_l \in \mathcal{Y}_l} \exp(-E_H(y_k, y_l)) \right)}_{r_{H \to Y_k}(y_k)} \cdot \underbrace{\left( \sum_{y_m \in \mathcal{Y}_m} \exp(-E_I(y_k, y_m)) \right)}_{r_{I \to Y_k}(y_k)} \right)$$

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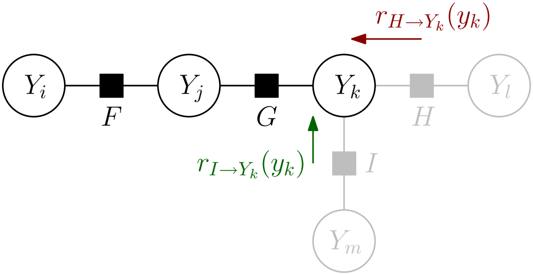


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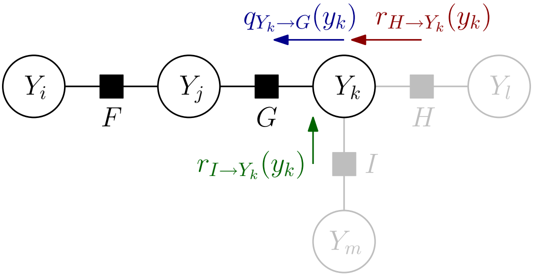


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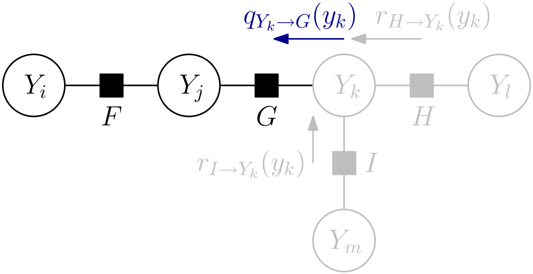


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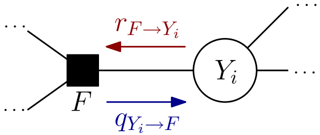
# Factor Graph Sum-Product Algorithm

- "Message": pair of vectors at each factor graph edge $(i, F) \in \mathcal{E}$
  1. $r_{F \to Y_i} \in \mathbb{R}^{\mathcal{Y}_i}$: factor-to-variable message
  2. $q_{Y_i \to F} \in \mathbb{R}^{\mathcal{Y}_i}$: variable-to-factor message
- Algorithm iteratively update messages
- After convergence: $Z$ and $\mu_F$ can be obtained from the messages



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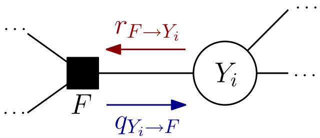


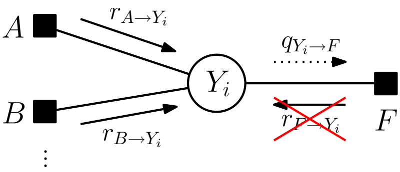
# Sum-Product: Variable-to-Factor message

- Set of factors adjacent to variable $i$

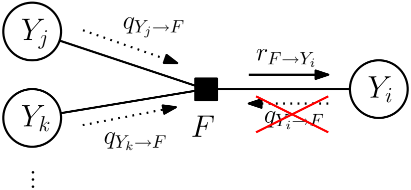
$$M(i) = \{F \in \mathcal{F} : (i, F) \in \mathcal{E}\}$$

- Variable-to-factor message

$$q_{Y_i \to F}(y_i) = \prod_{F' \in M(i) \setminus \{F\}} r_{F' \to Y_i}(y_i)$$



# Sum-Product: Factor-to-Variable message




- Factor-to-variable message

$$r_{F \to Y_i}(y_i) = \sum_{\substack{y'_F \in \mathcal{Y}_F, \\ y'_i = y_i}} \left( \exp\left(-E_F(y'_F)\right) \prod_{j \in N(F) \setminus \{i\}} q_{Y_j \to F}(y'_j) \right)$$

# Message Scheduling

$$q_{Y_i \to F}(y_i) = \prod_{F' \in M(i) \setminus \{F\}} r_{F' \to Y_i}(y_i)$$

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- Problem: message updates depend on each other
- No dependencies if product is empty $(= 1)$
- For tree-structured graphs we can resolve all dependencies

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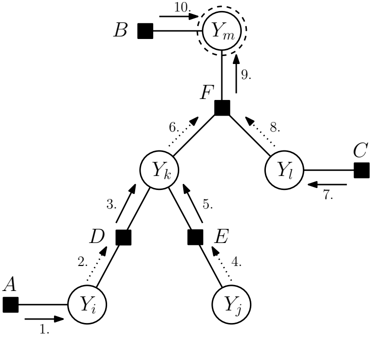
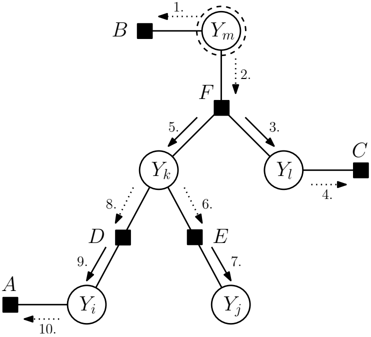
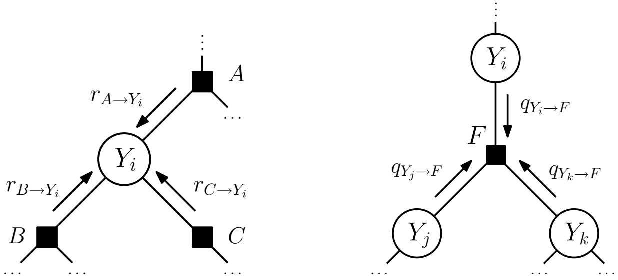
# Message Scheduling: Trees




1. Select one variable node as *tree root*
2. Compute leaf-to-root messages
3. Compute root-to-leaf messages

# Inference Results: $Z$ and marginals




- Partition function, evaluated at root

$$Z = \sum_{y_r \in \mathcal{Y}_r} \prod_{F \in M(r)} r_{F\to Y_r}(y_r)$$

- Marginal distributions, for each factor

$$\mu_F(y_F) = p(Y_F = y_F) = \frac{1}{Z} \exp\left(-E_F(y_F)\right) \prod_{i \in N(F)} q_{Y_i\to F}(y_i)$$

# Max-Product/Max-Sum Algorithm

- Belief Propagation for MAP inference

$$y^* = \operatorname*{argmax}_{y \in \mathcal{Y}} p(Y = y | x, w)$$

- Exact for trees
- For cyclic graphs: not as well understood as sum-product algorithm

$$\begin{aligned} q_{Y_i \to F}(y_i) &= \sum_{F' \in M(i) \setminus \{F\}} r_{F' \to Y_i}(y_i) \\ r_{F \to Y_i}(y_i) &= \max_{\substack{y'_F \in \mathcal{Y}_F, \\ y'_i = y_i}} \left( -E_F(y'_F) + \sum_{j \in N(F) \setminus \{i\}} q_{Y_j \to F}(y'_j) \right) \end{aligned}$$

# Sum-Product/Max-Sum comparison

Sum-Product

$$
\begin{aligned}
q_{Y_i \to F}(y_i) &= \prod_{F' \in M(i) \setminus \{F\}} r_{F' \to Y_i}(y_i) \\
r_{F \to Y_i}(y_i) &= \sum_{\substack{y'_F \in \mathcal{Y}_F, \\ y'_i = y_i}} \left( \exp\left(-E_F(y'_F)\right) \prod_{j \in N(F) \setminus \{i\}} q_{Y_j \to F}(y'_j) \right)
\end{aligned}
$$

Max-Sum

$$
\begin{aligned}
q_{Y_i \to F}(y_i) &= \sum_{F' \in M(i) \setminus \{F\}} r_{F' \to Y_i}(y_i) \\
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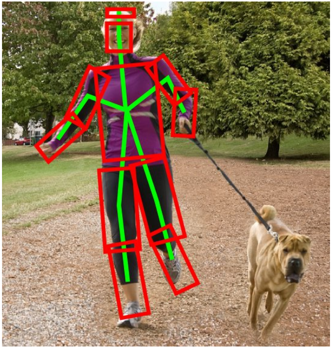
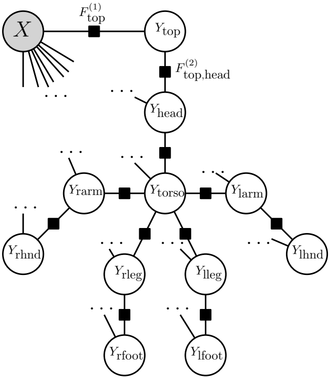
# Example: Pictorial Structures






- Tree-structured model for articulated pose (Felzenszwalb and Huttenlocher, 2000), (Fischler and Elschlager, 1973)
- Body-part variables, states: discretized tuple $(x, y, s, \theta)$
- $(x, y)$ position, $s$ scale, and $\theta$ rotation

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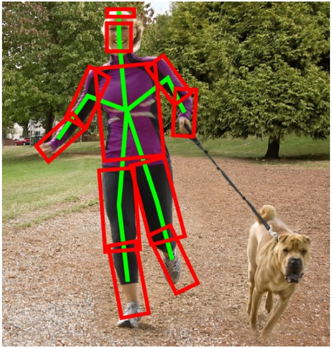

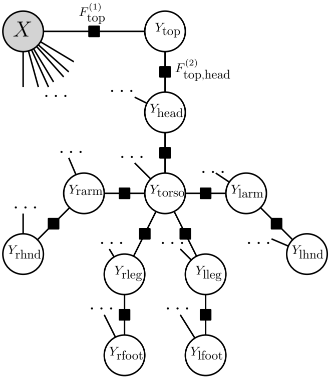


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- $(x, y)$ position, $s$ scale, and $\theta$ rotation

# Example: Pictorial Structures (cont)

$$r_{F\to Y_i}(y_i) \quad = \max_{\substack{(y_i',y_j')\in\mathcal{Y}_i\times\mathcal{Y}_j,\\ y_i'=y_i}} \left( -E_F(y_i',y_j') + \sum_{j\in N(F)\setminus\{i\}} q_{Y_j\to F}(y_j') \right) \quad (1)$$

- Because $\mathcal{Y}_i$ is large ($\approx 500k$), $\mathcal{Y}_i \times \mathcal{Y}_j$ is too big
- (Felzenszwalb and Huttenlocher, 2000) use special form for $E_F(y_i, y_j)$ so that (1) is computable in $O(|\mathcal{Y}_i|)$

# Loopy Belief Propagation

- Key difference: no schedule that removes dependencies
- But: message computation is still well defined
- Therefore, classic loopy belief propagation (Pearl, 1988)
  1. Initialize message vectors to 1 (sum-product) or 0 (max-sum)
  2. Update messages, hoping for convergence
  3. Upon convergence, treat beliefs $\mu_F$ as approximate marginals
- Different messaging schedules (synchronous/asynchronous, static/dynamic)
- Improvements: generalized BP (Yedidia et al., 2001), convergent BP (Heskes, 2006)

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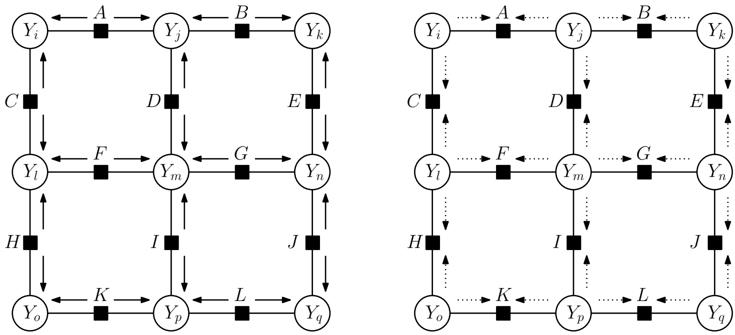
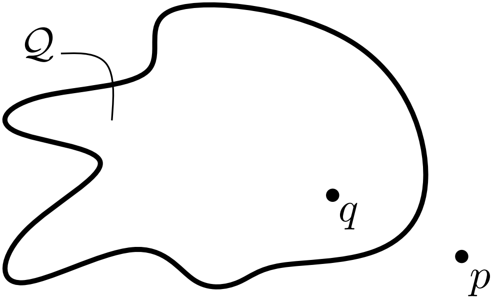
# Synchronous Iteration



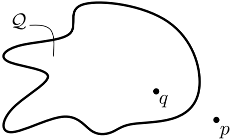
# Mean field methods

- Mean field methods (Jordan et al., 1999), (Xing et al., 2003)
- Distribution $p(y|x, w)$, inference intractable
- Approximate distribution $q(y)$
- Tractable family $\mathcal{Q}$



# Mean field methods (cont)

$$q^* = \operatorname*{argmin}_{q \in \mathcal{Q}} D_{KL}(q(y) \| p(y|x,w))$$




$$\begin{aligned} & D_{KL}(q(y) \| p(y|x,w)) \\ = & \sum_{y \in \mathcal{Y}} q(y) \log \frac{q(y)}{p(y|x,w)} \\ = & \sum_{y \in \mathcal{Y}} q(y) \log q(y) - \sum_{y \in \mathcal{Y}} q(y) \log p(y|x,w) \\ = & -H(q) + \sum_{F \in \mathcal{F}} \sum_{y_F \in \mathcal{Y}_F} \mu_{F,y_F}(q) E_F(y_F; x_F, w) + \log Z(x,w), \end{aligned}$$

where $H(q)$ is the *entropy* of $q$ and $\mu_{F,y_F}$ are the marginals of $q$. (The form of $\mu$ depends on $\mathcal{Q}$.)

# Mean field methods (cont)

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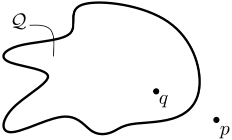


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# Mean field methods (cont)

$$q^* = \operatorname*{argmin}_{q \in \mathcal{Q}} D_{KL}(q(y) \| p(y|x, w))$$

- When $\mathcal{Q}$ is rich: $q^*$ is close to $p$
- Marginals of $q^*$ approximate marginals of $p$
- *Gibbs inequality*

$$D_{KL}(q(y) \| p(y|x, w)) \geq 0$$

- Therefore, we have a lower bound

$$\log Z(x, w) \geq H(q) - \sum_{F \in \mathcal{F}} \sum_{y_F \in \mathcal{Y}_F} \mu_{F, y_F}(q) E_F(y_F; x_F, w).$$

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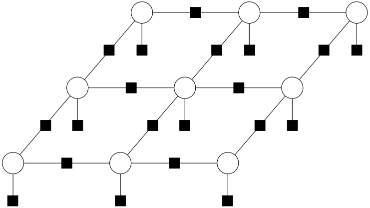
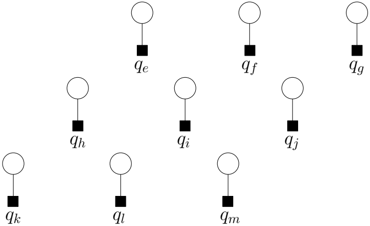
# Naive Mean Field

- Set $\mathcal{Q}$ all distributions of the form

$$q(y) = \prod_{i \in V} q_i(y_i).$$





# Naive Mean Field

- Set $\mathcal{Q}$ all distributions of the form

$$q(y) = \prod_{i \in V} q_i(y_i).$$

- Marginals $\mu_{F,y_F}$ take the form

$$\mu_{F,y_F}(q) = \prod_{i \in N(F)} q_i(y_i).$$

- Entropy $H(q)$ decomposes

$$H(q) = \sum_{i \in V} H_i(q_i) = -\sum_{i \in V} \sum_{y_i \in \mathcal{Y}_i} q_i(y_i) \log q_i(y_i).$$

# Naive Mean Field (cont)

Putting it together,

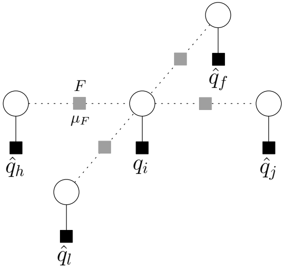
$$
\begin{aligned}
& \operatorname*{argmin}_{q \in \mathcal{Q}} \quad D_{KL}(q(y) \| p(y|x,w)) \\
= & \operatorname*{argmax}_{q \in \mathcal{Q}} \quad H(q) - \sum_{F \in \mathcal{F}} \sum_{y_F \in \mathcal{Y}_F} \mu_{F,y_F}(q) E_F(y_F; x_F, w) - \log Z(x,w) \\
= & \operatorname*{argmax}_{q \in \mathcal{Q}} \quad H(q) - \sum_{F \in \mathcal{F}} \sum_{y_F \in \mathcal{Y}_F} \mu_{F,y_F}(q) E_F(y_F; x_F, w) \\
= & \operatorname*{argmax}_{q \in \mathcal{Q}} \quad \Bigg[ - \sum_{i \in V} \sum_{y_i \in \mathcal{Y}_i} q_i(y_i) \log q_i(y_i) \\
& \qquad - \sum_{F \in \mathcal{F}} \sum_{y_F \in \mathcal{Y}_F} \Big( \prod_{i \in N(F)} q_i(y_i) \Big) E_F(y_F; x_F, w) \Bigg].
\end{aligned}
$$

Optimizing over $\mathcal{Q}$ is optimizing over $q_i \in \Delta_i$, the probability simplices.

# Naive Mean Field (cont)

$$\operatorname*{argmax}_{q \in \mathcal{Q}} \left[ -\sum_{i \in V} \sum_{y_i \in \mathcal{Y}_i} q_i(y_i) \log q_i(y_i) - \sum_{F \in \mathcal{F}} \sum_{y_F \in \mathcal{Y}_F} \left( \prod_{i \in N(F)} q_i(y_i) \right) E_F(y_F; x_F, w) \right].$$

- Non-concave maximization problem $\rightarrow$ hard. (For general $E_F$ and pairwise or higher-order factors.)
- Block coordinate ascent: closed-form update for each $q_i$



# Naive Mean Field (cont)

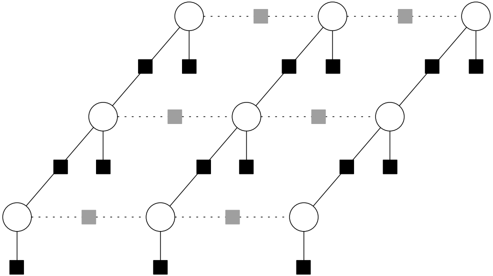
Closed form update for $q_i$:

$$
\begin{aligned}
q_i^*(y_i) &= \exp\left(1 - \sum_{\substack{F\in\mathcal{F},\\ i\in N(F)}} \sum_{\substack{y_F\in\mathcal{Y}_F,\\ [y_F]_i=y_i}} \left(\prod_{j\in N(F)\setminus\{i\}} \hat{q}_j(y_j)\right) E_F(y_F; x_F, w) + \lambda\right) \\
\lambda &= -\log\left(\sum_{y_i\in\mathcal{Y}_i} \exp\left(1 - \sum_{\substack{F\in\mathcal{F},\\ i\in N(F)}} \sum_{\substack{y_F\in\mathcal{Y}_F,\\ [y_F]_i=y_i}} \left(\prod_{j\in N(F)\setminus\{i\}} \hat{q}_j(y_j)\right) E_F(y_F; x_F, w)\right)\right)
\end{aligned}
$$

- Look scary, but very easy to implement

# Structured Mean Field

- Naive mean field approximation can be poor
- Structured mean field (Saul and Jordan, 1995) uses factorial approximations with larger tractable subgraphs
- Block coordinate ascent: optimizing an entire subgraph using exact probabilistic inference on trees



# Sampling

Probabilistic inference and related tasks require the computation of

$$\mathbb{E}_{y \sim p(y|x,w)}[h(x,y)],$$

where $h : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ is an arbitary but well-behaved function.

- Inference: $h_{F,z_F}(x,y) = I(y_F = z_F)$,

  $$\mathbb{E}_{y \sim p(y|x,w)}[h_{F,z_F}(x,y)] = p(y_F = z_F | x, w),$$

  the marginal probability of factor $F$ taking state $z_F$.
- Parameter estimation: *feature map* $h(x,y) = \phi(x,y)$, $\phi : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}^d$,

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  "expected *sufficient statistics* under the model distribution".

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# Monte Carlo

- Sample approximation from $y^{(1)}, y^{(2)}, \ldots$

$$\mathbb{E}_{y \sim p(y|x,w)}[h(x,y)] \approx \frac{1}{S} \sum_{s=1}^{S} h(x, y^{(s)}).$$

- When the expectation exists, then the *law of large numbers* guarantees convergence for $S \to \infty$,
- For $S$ independent samples, approximation error is $O(1/\sqrt{S})$, *independent* of the dimension $d$.

Problem

- Producing exact samples $y^{(s)}$ from $p(y|x)$ is *hard*

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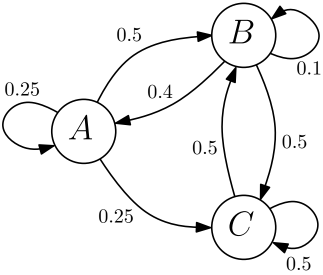
# Markov Chain Monte Carlo (MCMC)

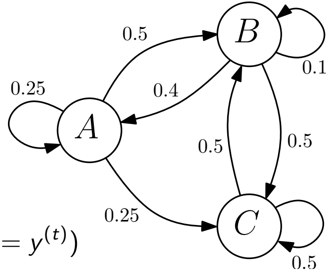
- *Markov chain* with $p(y|x)$ as stationary distribution
- Here: $\mathcal{Y} = \{A, B, C\}$
- Here: $p(y) = (0.1905, 0.3571, 0.4524)$



# Markov Chains

## Definition (Finite Markov chain)

Given a finite set $\mathcal{Y}$ and a matrix $P \in \mathbb{R}^{\mathcal{Y}\times\mathcal{Y}}$, then a random process $(Z_1, Z_2, \ldots)$ with $Z_t$ taking values from $\mathcal{Y}$ is a *Markov chain with transition matrix P*, if




$$\begin{aligned} & p(Z_{t+1} = y^{(j)} | Z_1 = y^{(1)}, Z_2 = y^{(2)}, \ldots, Z_t = y^{(t)}) \\ = \; & p(Z_{t+1} = y^{(j)} | Z_t = y^{(t)}) \\ = \; & P_{y^{(t)}, y^{(j)}} \end{aligned}$$

# MCMC Simulation (1)

Steps

1. Construct a Markov chain with stationary distribution $p(y|x,w)$
2. Start at $y^{(0)}$
3. Perform random walk according to Markov chain
4. After sufficient number $S$ of steps, stop and treat $y^{(S)}$ as sample from $p(y|x,w)$

- Justified by *ergodic theorem*.
- In practise: discard a fixed number of initial samples ("burn-in phase") to forget starting point
- In practise: afterwards, use between $100$ to $100,000$ samples

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# Gibbs sampler

How to construct a suitable Markov chain?

- *Metropolis-Hastings chain*, almost always possible
- Special case: *Gibbs sampler* (Geman and Geman, 1984)
  1. Select a variable $y_i$,
  2. Sample $y_i \sim p(y_i | y_{V \setminus \{i\}}, x)$.

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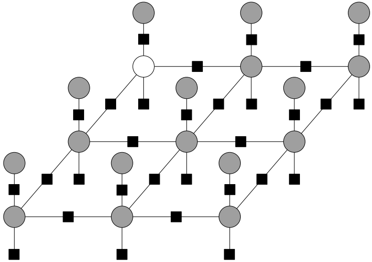
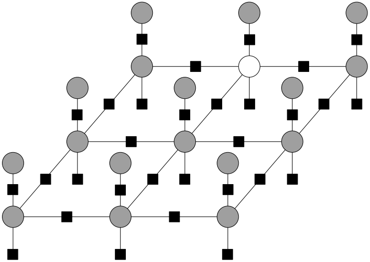
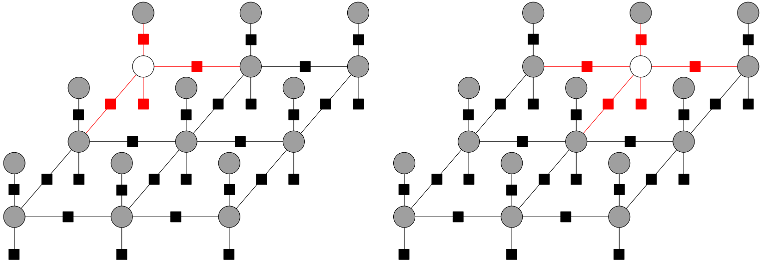
# Gibbs Sampler

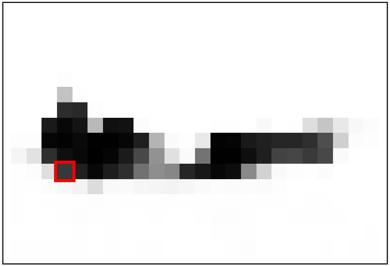
$$p(y_i | y^{(t)}_{V \setminus \{i\}}, x, w) = \frac{p(y_i, y^{(t)}_{V \setminus \{i\}} | x, w)}{\sum_{y_i \in \mathcal{Y}_i} p(y_i, y^{(t)}_{V \setminus \{i\}} | x, w)} = \frac{\tilde{p}(y_i, y^{(t)}_{V \setminus \{i\}} | x, w)}{\sum_{y_i \in \mathcal{Y}_i} \tilde{p}(y_i, y^{(t)}_{V \setminus \{i\}} | x, w)}$$

# Gibbs Sampler



$$p(y_i|y^{(t)}_{V\setminus\{i\}}, x, w) = \frac{\sum_{F \in M(i)} \exp(-E_F(y_i, y^{(t)}_{F\setminus\{i\}}, x_F, w))}{\sum_{y_i \in \mathcal{Y}_i} \sum_{F \in M(i)} \exp(-E_F(y_i, y^{(t)}_{F\setminus\{i\}}, x_F, w))}$$

# Example: Gibbs sampler



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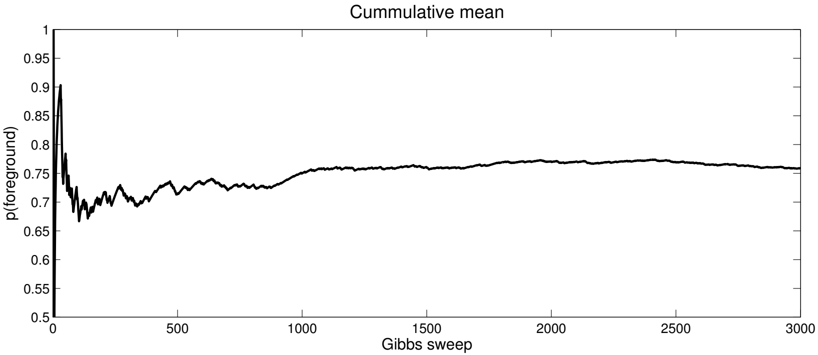

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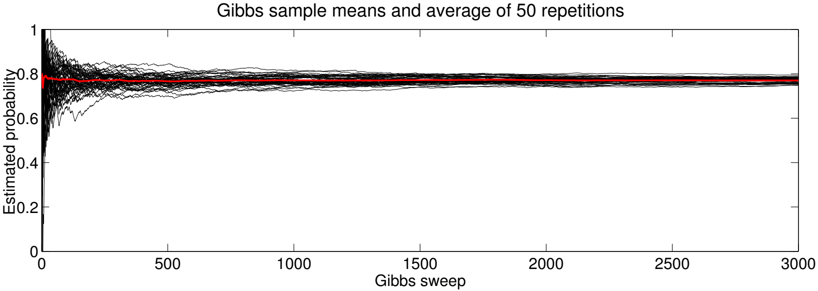
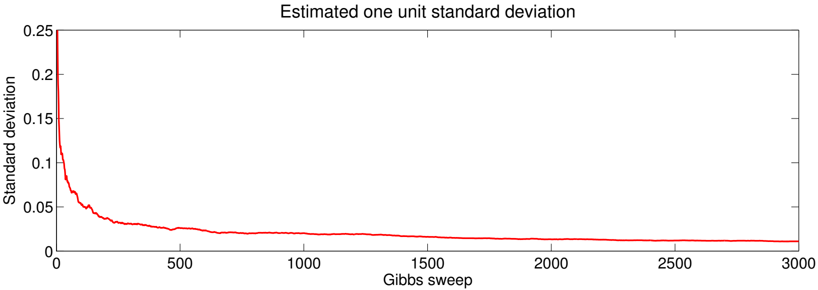


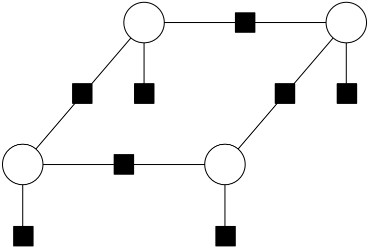

- $p(y_i = \text{``}foreground\text{''}) \approx 0.770 \pm 0.011$

# Example: Gibbs sampler

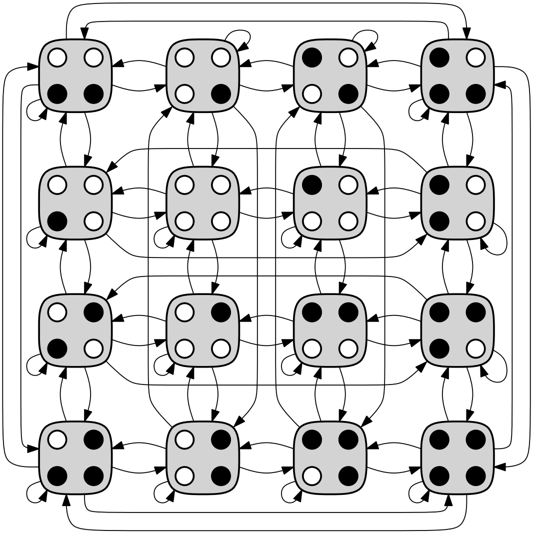



- Standard deviation $O(1/\sqrt{S})$

# Gibbs Sampler Transitions



# Gibbs Sampler Transitions

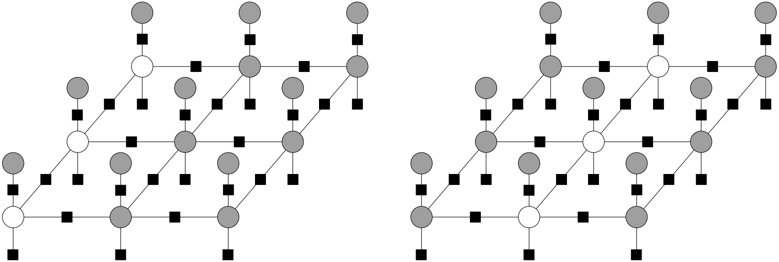


# Block Gibbs Sampler

Extension to larger groups of variables

1. Select a block $y_I$
2. Sample $y_I \sim p(y_I | y_{V \setminus I}, x)$

$\rightarrow$ Tractable if sampling from blocks is tractable.



# Summary: Sampling

Two families of Monte Carlo methods

1. Markov Chain Monte Carlo (MCMC)
2. Importance Sampling

Properties

- Often simple to implement, general, parallelizable
- (Cannot compute partition function $Z$)
- Can fail without any warning signs

References

- (Häggström, 2000), introduction to Markov chains
- (Liu, 2001), excellent Monte Carlo introduction

# Coffee Break

## Coffee Break

Continuing at 10:30am

Slides available at
`http://www.nowozin.net/sebastian/cvpr2011tutorial/`