CSC535: Probabilistic Graphical Models

Final Exam Review

Prof. Jason Pacheco

Administrative Items

- Final will be out Tuesday, 12/10
- Due 12/18 @ 11:59pm
- 4 questions (20 points) + Extra Credit (1 point)
- **You may provide handwritten responses (scanned PDF)**
- Make sure handwriting is clear and easy-to-read

Topics

- Probability and Statistics
- Probabilistic Graphical Models
- Message Passing Inference
- Parameter Learning
- Monte Carlo Methods

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Probability and Random Events

Fundamental Rules of Probability

- Conditional: $p(X \mid Y) = \frac{p(X,Y)}{p(Y)} = \frac{p(X,Y)}{\sum_x p(X=x,Y)}$
- Law of total probability: $p(Y) = \sum_x p(Y, X = x)$
- Probability chain rule: $p(X, Y) = p(Y)p(X \mid Y)$

Independence of RVs

- Two RVs X & Y are independent iff: $p(X \mid Y) = p(X)$
- Equivalently: $p(X, Y) = p(X)p(Y)$
- X & Y are conditionally independent given Z iff: $p(X \mid Y, Z) = p(X \mid Z)$
- Equivalently: $p(X, Y \mid Z) = p(X \mid Z)p(Y \mid Z)$

Tabular Method

Let X, Y be binary RVs with the joint probability table

For Binomial use K-by-K probability table.

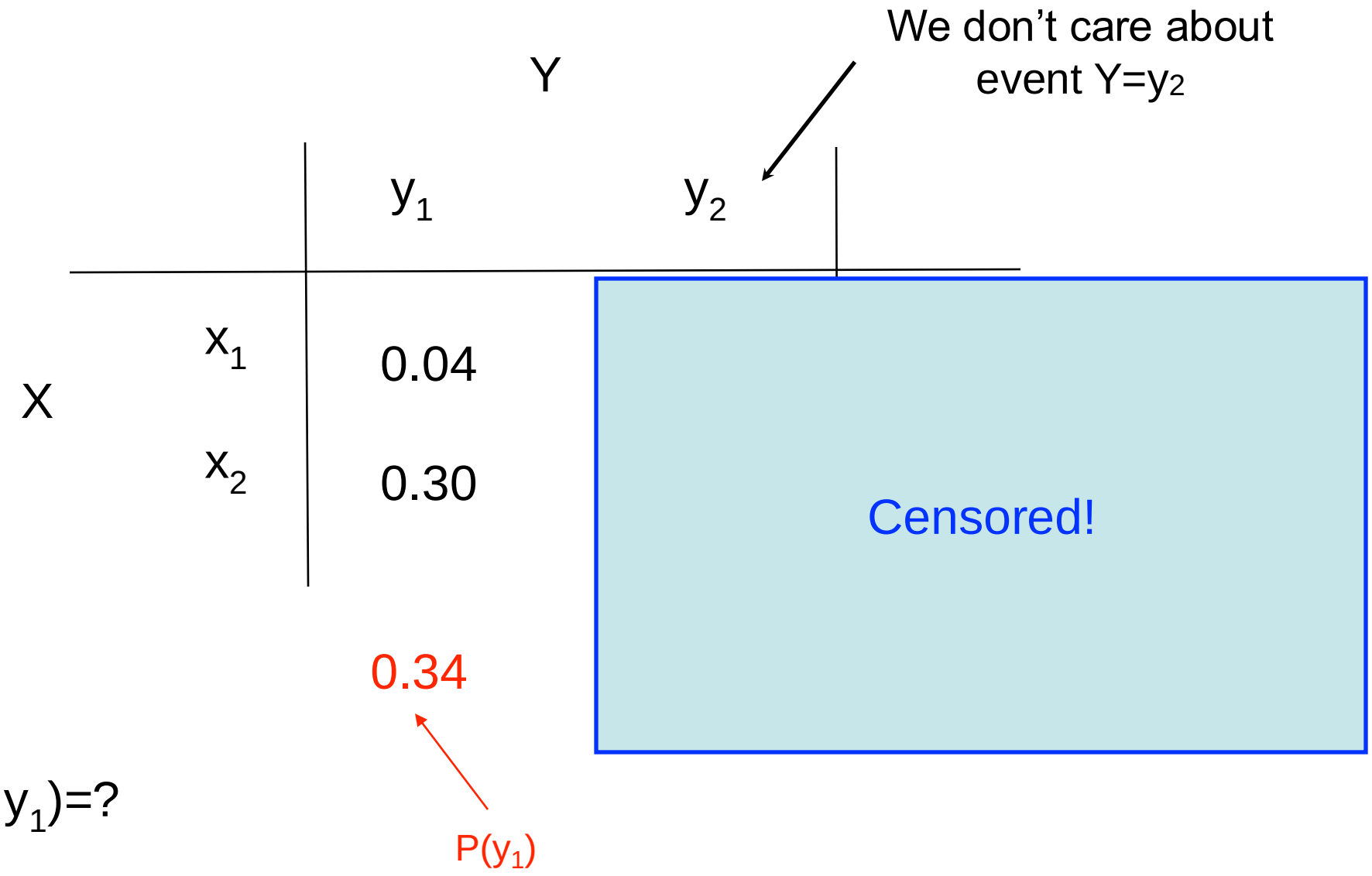
X \ Y	y_1	y_2	
x_1	0.04	0.36	0.4
x_2	0.30	0.30	0.6
	0.34	0.66	

$P(x_1)$, $P(x_2)$, $P(x)$, $P(y)$, $P(y_1)$, $P(y_2)$

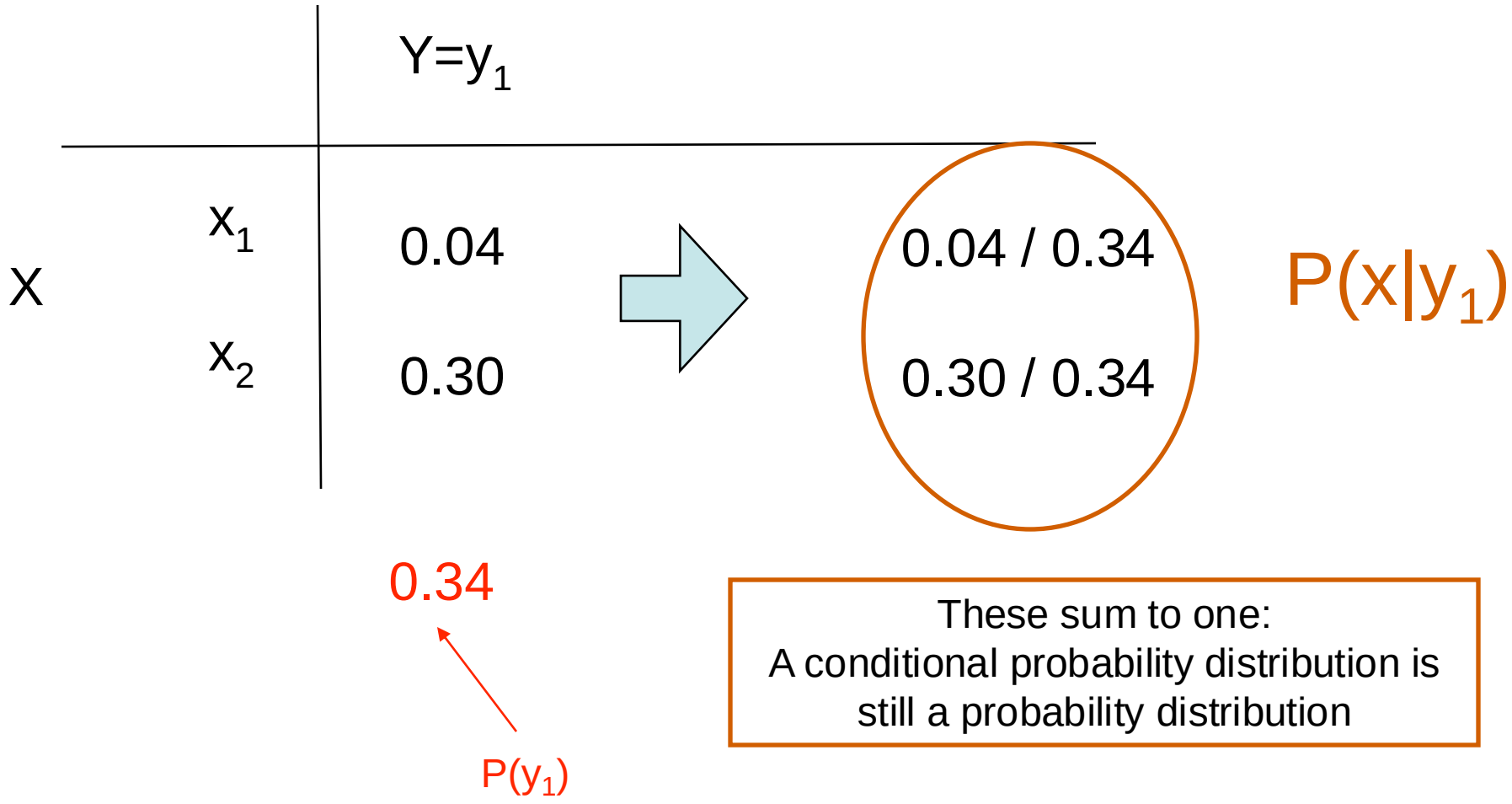
$P(y_1)=P(x_1,y_1)+P(x_2,y_1)$
$P(y_2)=P(x_1,y_2)+P(x_2,y_2)$
[i.e., sum down columns]

$P(x_1)=P(x_1,y_1)+P(x_1,y_2)$
$P(x_2)=P(x_2,y_1)+P(x_2,y_2)$
[i.e., sum across rows]

Tabular Method

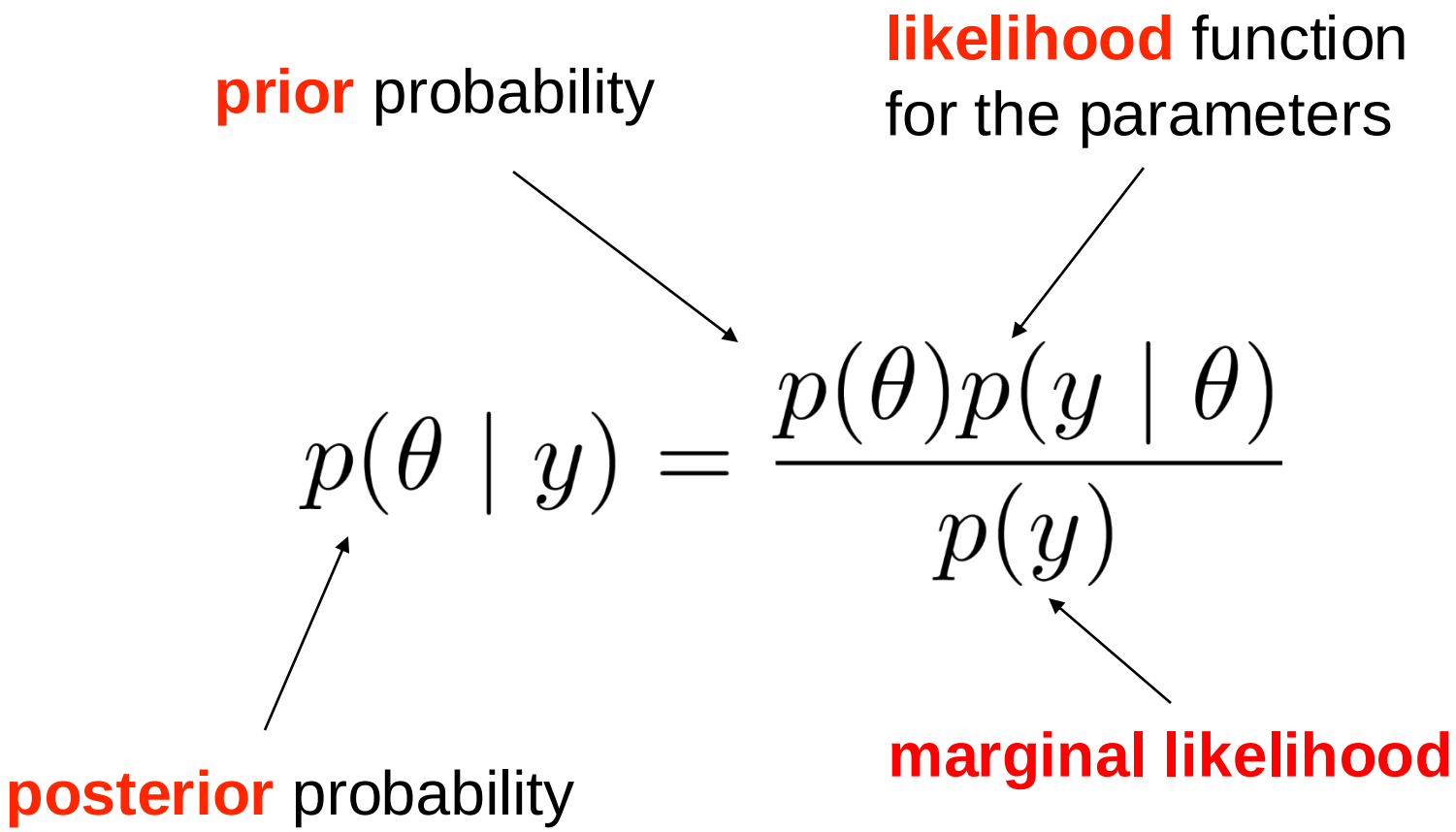


Tabular Method



Bayes' Rule

Posterior represents all uncertainty <u>after</u> observing data…



Bayesian Inference Example

About 29% of American adults have high blood pressure (BP). Home test has 30% false positive rate and no false negative error.

A recent home test states that you have high BP. Should you start medication?

An Assessment of the Accuracy of Home Blood Pressure Monitors When Used in Device Owners

Jennifer S. Ringrose,[1] Gina Polley,[1] Donna McLean,[2–4] Ann Thompson,[1,5] Fraulein Morales,[1] and Raj Padwal[1,4,6]

Bayesian Inference Example

About 29% of American adults have high blood pressure (BP). Home test has 30% false positive rate and no false negative error.

- Latent quantity of interest is hypertension: $\theta \in \{true, false\}$
- Measurement of hypertension: $y \in \{true, false\}$
- Prior: $p(\theta = true) = 0.29$
- Likelihood: $p(y = true \mid \theta = false) = 0.30$

$$p(y = true \mid \theta = true) = 1.00$$

Bayesian Inference Example

About 29% of American adults have high blood pressure (BP). Home test has 30% false positive rate and no false negative error.

Suppose we get a positive measurement, then posterior is:

$$p(\theta = true \mid y = true) = \frac{p(\theta = true)p(y = true \mid \theta = true)}{p(y = true)}$$

$$= \frac{0.29 * 1.00}{0.29 * 1.00 + 0.71 * 0.30} \approx 0.58$$

Bayesian Estimation

Task: *produce an estimate* $\hat{\theta}$ *of* θ *after observing data* y

Bayes estimators minimize expected **loss function**:

$$\mathbb{E}[L(\theta, \hat{\theta}) \mid y] = \int p(\theta \mid y) L(\theta, \hat{\theta})\, d\theta$$

Example: Minimum mean squared error (MMSE):

$$\hat{\theta}^{\mathrm{MMSE}} = \arg\min \mathbb{E}[(\hat{\theta} - \theta)^2 \mid y] = E[\theta \mid y]$$

Posterior mean always minimizes squared error.

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Directed Graphical Models

- Distribution factorized as product of conditionals via chain rule

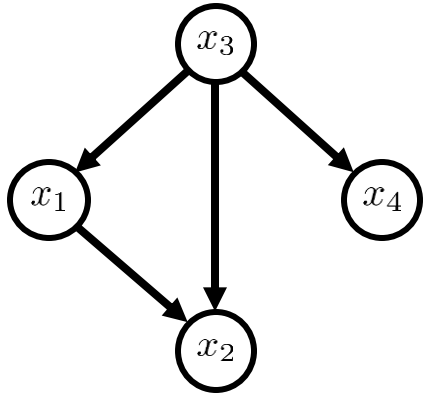
$$p(x_1, x_2, x_3, x_4) = p(x_3)p(x_1 \mid x_3)p(x_4 \mid x_1, x_3)p(x_2 \mid x_1, x_3, x_4)$$

- Choose ordering where terms simplify due to conditional independence

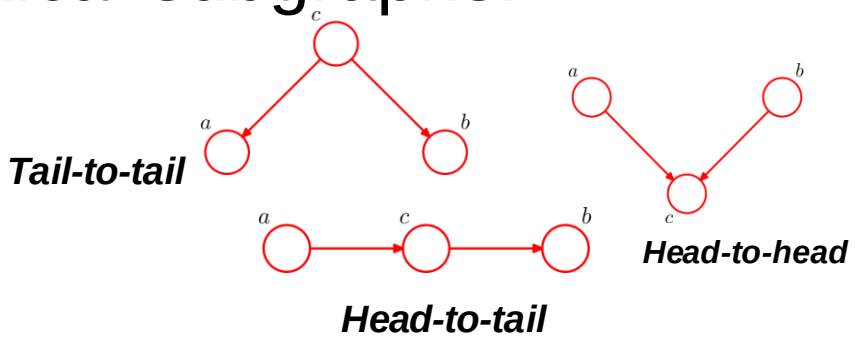
Eg. Suppose $x_4 \perp x_1 \mid x_3$ and $x_2 \perp x_4 \mid x_1$ then:

$$p(x) = p(x_3)p(x_1 \mid x_3)p(x_4 \mid x_3)p(x_2 \mid x_1, x_3)$$

- Directed graph encodes factorized distribution via conditional independence properties

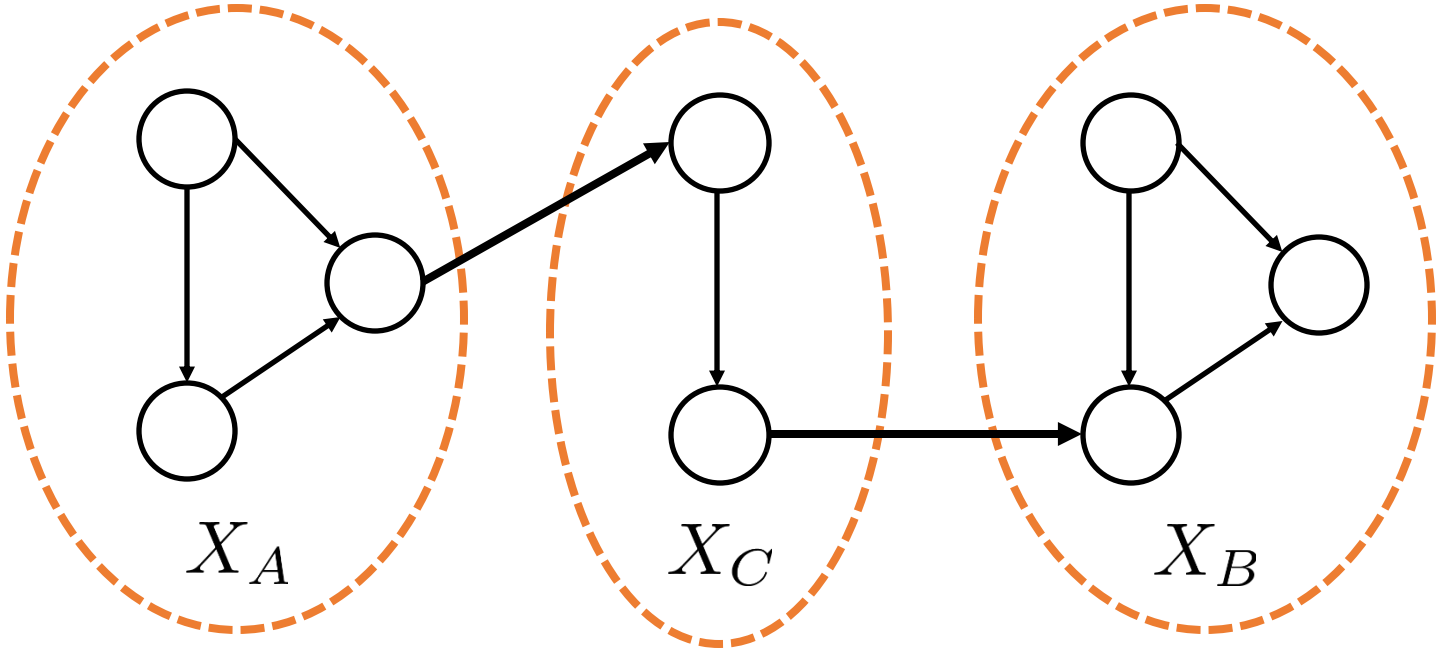


- Test independence using canonical subgraphs:
- Straightforward simulation via **ancestral sampling**



Bayes Ball Algorithm

To test if $X_A \perp X_B \mid X_C$ roll ball from *every node in* X_A …



If *any* ball reaches *any node* in X_B then

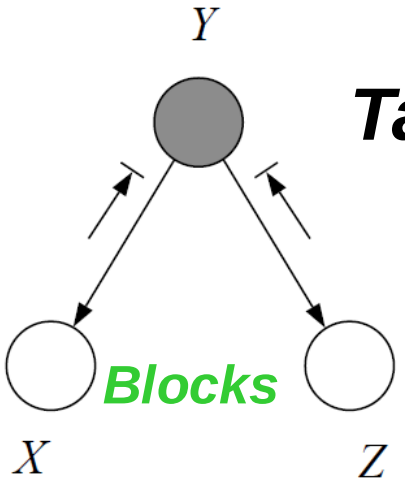
$$X_A \not\perp X_B \mid X_C$$

Otherwise:

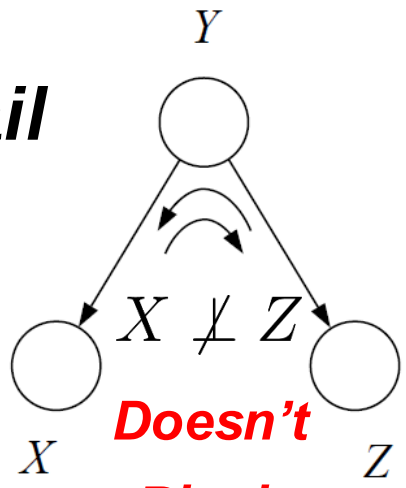
$$X_A \perp X_B \mid X_C$$

Tests for property of ***directed separation*** **(d-separation)**: if X_C separates / blocks X_A from X_B then $X_A \perp X_B \mid X_C$

Bayes Ball Algorithm



Tail-to-Tail

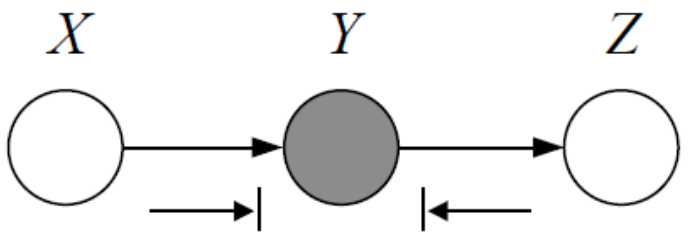


Blocks

$$X \perp Z \mid Y$$

$$X \not\perp Z$$

Doesn't Block

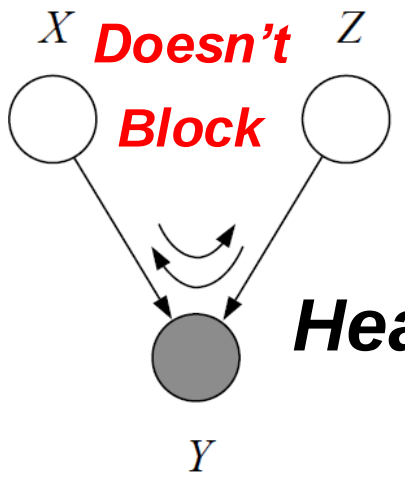


Blocks

$$X \perp Z \mid Y$$

Head-to-Tail

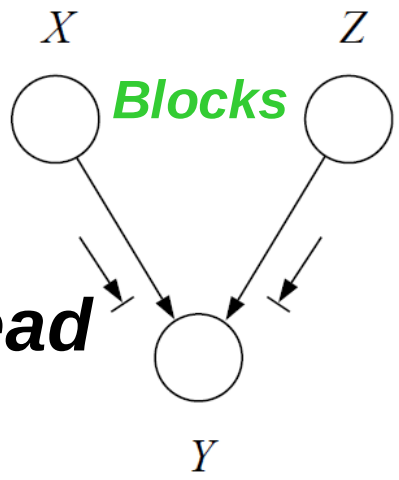
$$X \not\perp Z \mid Y$$



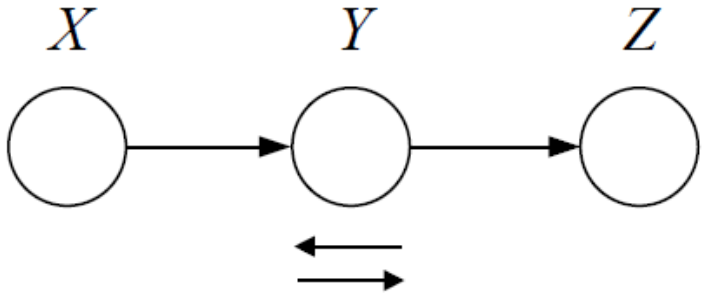
Doesn't Block

Head-to-Head

$$X \perp Z$$



Blocks



Doesn't Block

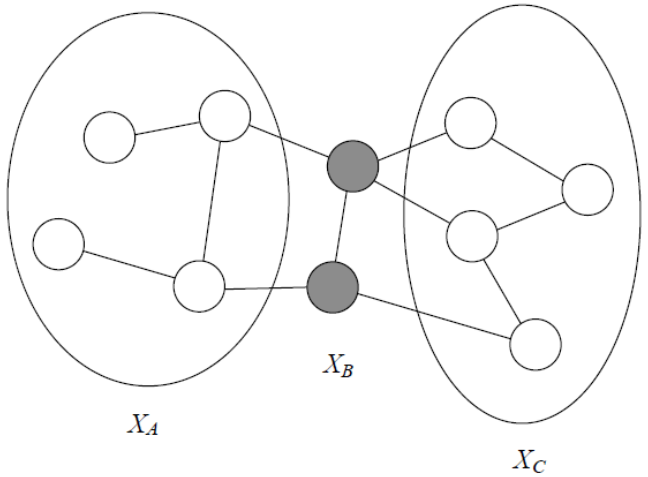
$$X \not\perp Z$$

Undirected Graphical Models

- Joint factorization as nonnegative factors (potentials) over subsets:

$$p(x) \propto \prod_{f \in \mathcal{F}} \psi_f(x_f)$$

- Easier to specify models compared to Bayes nets since:
  - Factors do not need to be normalized conditional probabilities
  - May specify up to unknown normalization constant
- Easier to verify Markov independence via *separating sets*
- Factorization ambiguous in MRFs, but explicit in factor graphs (factor graphs generally preferred)
- Simulation is not easy in general. Can't do ancestral sampling.

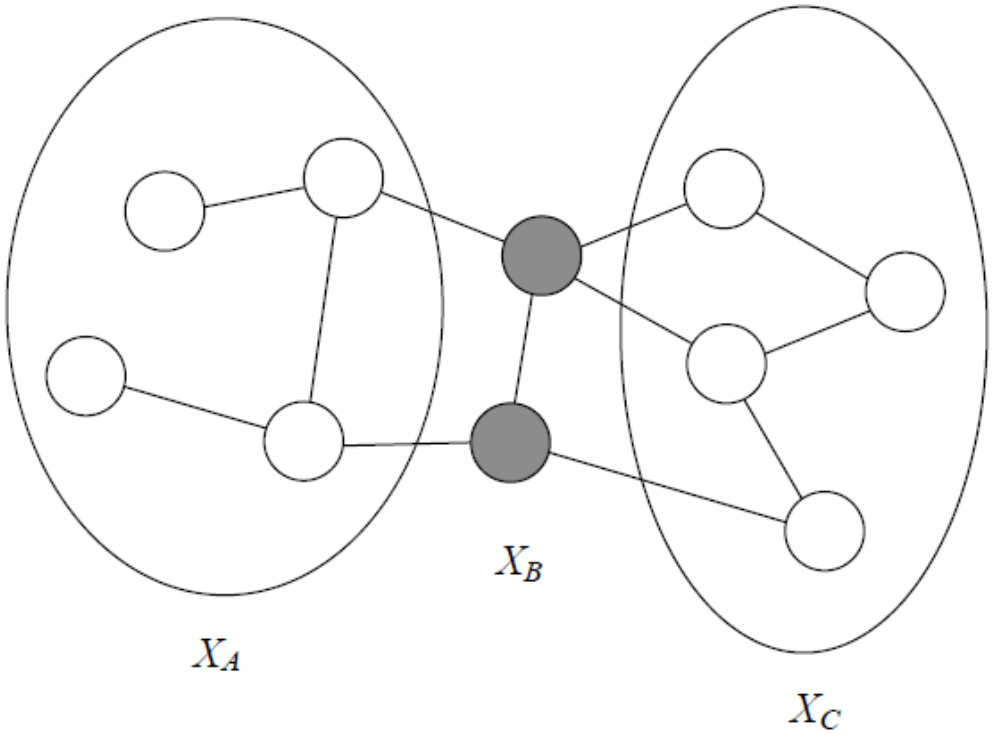


Conditional Independence (Undirected)

We say x_A and x_C are conditionally *independent* $x_A \perp\!\!\!\perp x_C \mid x_B$ *given variables* x_B *iff,*

$$p(x_A, x_C \mid x_B) = p(x_A \mid x_B)p(x_C \mid x_B)$$

Def. We say $p(x)$ is *globally Markov* w.r.t. $\mathcal{G}$ if $x_A \perp\!\!\!\perp x_C \mid x_B$ in any separating set of $\mathcal{G}$.

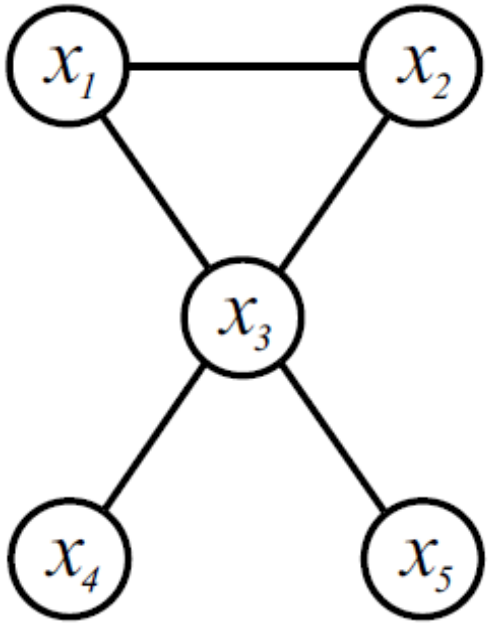


Conditional independence in undirected graphical models is defined by separating sets

[Source: Michael I. Jordan]

Markov Random Fields (MRFs)

A factor $\psi_c(x_c)$ corresponds to a clique $c \in \mathcal{C}$ (fully connected subgraph) in the MRF



An MRF does not imply a unique factorization, for example either of the following are "*valid*":

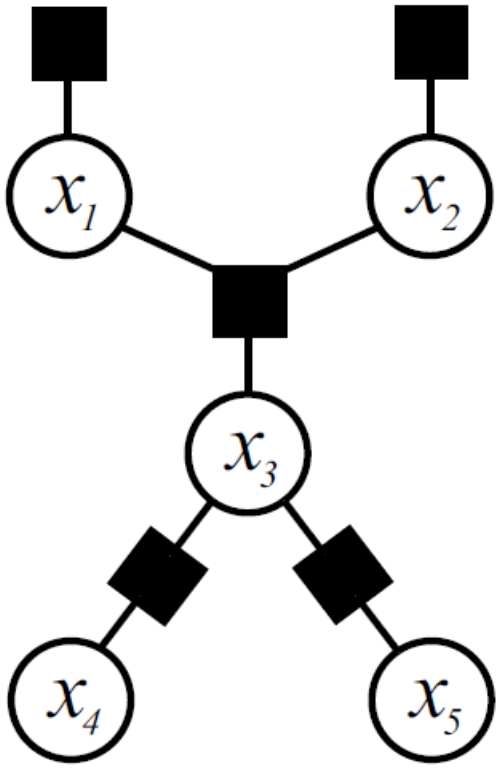
$$\psi(x_1, x_2, x_3)\psi(x_3, x_4)\psi(x_3, x_5)$$

$$\psi(x_1, x_2)\psi(x_2, x_3)\psi(x_1, x_3)\psi(x_3, x_4)\psi(x_3, x_5)$$

A factorization is *valid* if it satisfies the *Global Markov property*, defined by conditional independencies

Factor Graphs

Factor graphs make factorization explicit…



Factor node for each product term in the joint factorization:

$$p(x) \propto \prod_{f \in \mathcal{F}} \psi_f(x_f)$$

where $x_f = \{x_i : i \in f\}$ the set of variables in factor *f*. For example:

$$\psi(x_1)\psi(x_2)\psi(x_1, x_2, x_3)\psi(x_3, x_4)\psi(x_3, x_5)$$

Factor nodes correspond to MRF cliques

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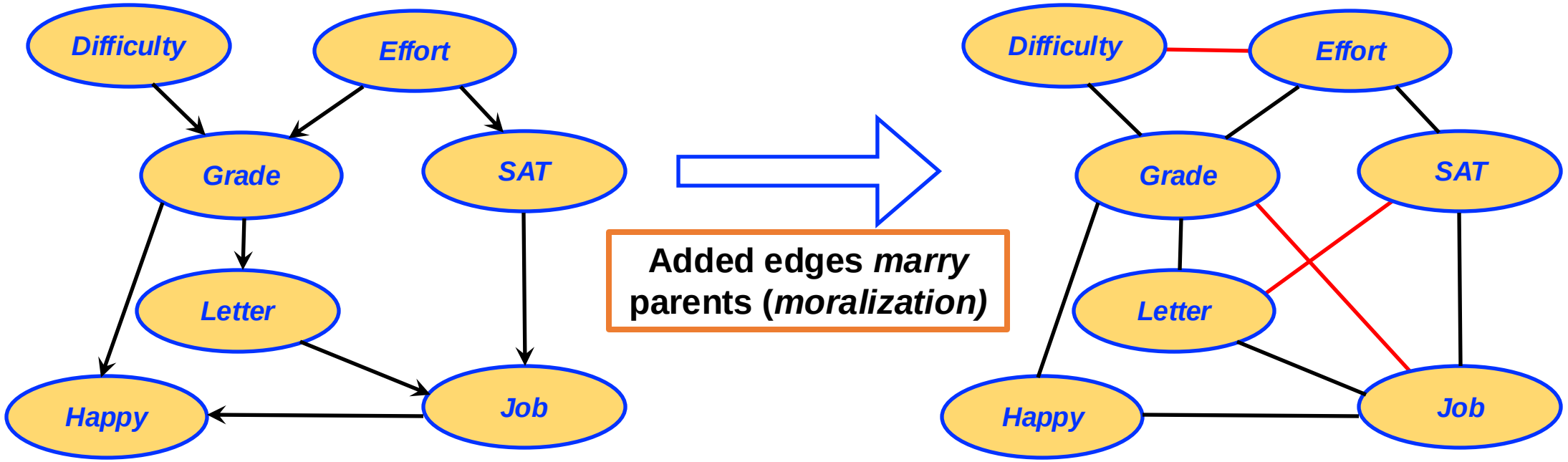
Bayes Net → MRF



$$P(\cdot) = P(D)P(E)P(G \mid D, E)P(S \mid E)P(L \mid G)P(J \mid S, L)P(H \mid J, G)$$

Drop local normalization

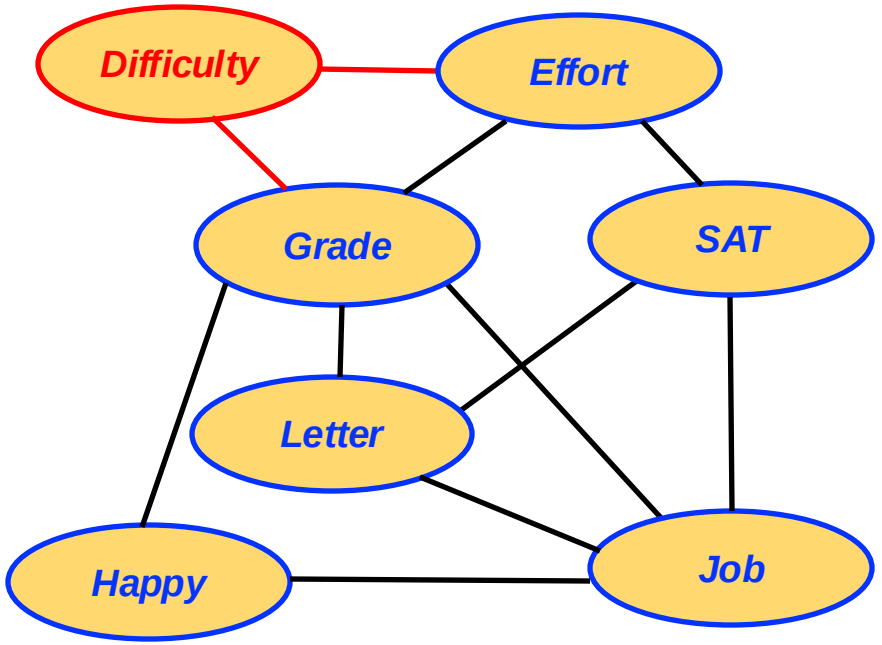
$$P(\cdot) \propto \psi(D)\psi(E)\psi(G, D, E)\psi(S, E)\psi(L, G)\psi(J, S, L)\psi(H, J, G)$$

Variable Elimination

Elimination order D, E, H, G, S, L

Worst-case Complexity:

$\mathcal{O}(K^3)$



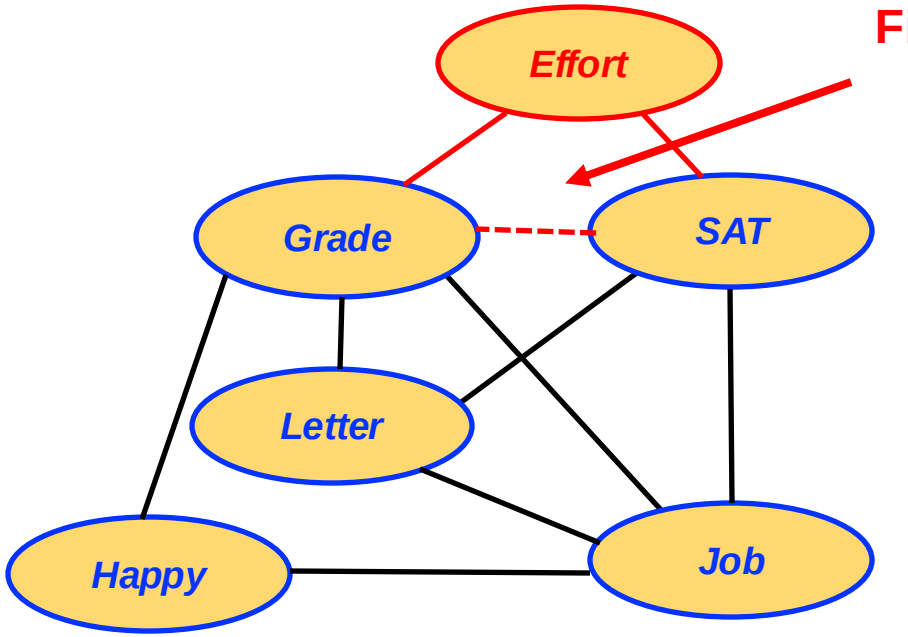
$$\phi(D, E, G) = \mathcal{O}(K^3)$$

Variable Elimination

Elimination order D, E, H, G, S, L

Worst-case Complexity:

$$\mathcal{O}(K^3)$$



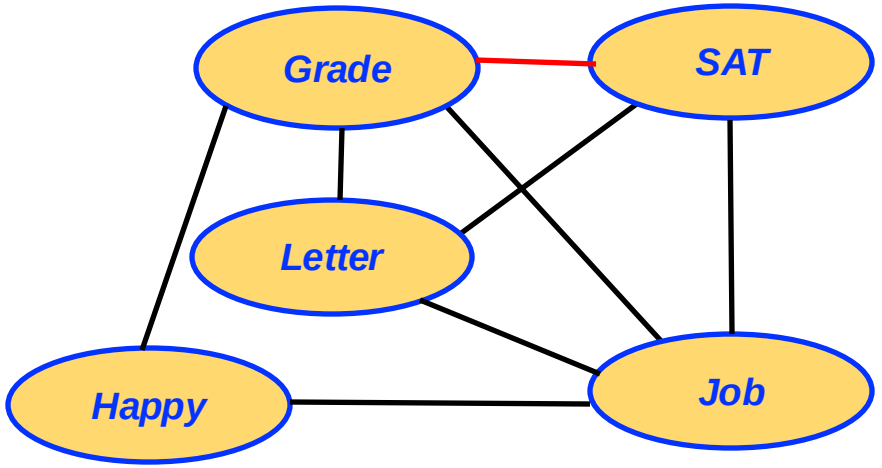
Fill-in edge since Effort passes message to Grade and SAT

$$\phi(E, G, S) = \mathcal{O}(K^3)$$

Variable Elimination

Elimination order D, E, H, G, S, L

Fill-in Edge



Worst-case Complexity:

$\mathcal{O}(K^3)$

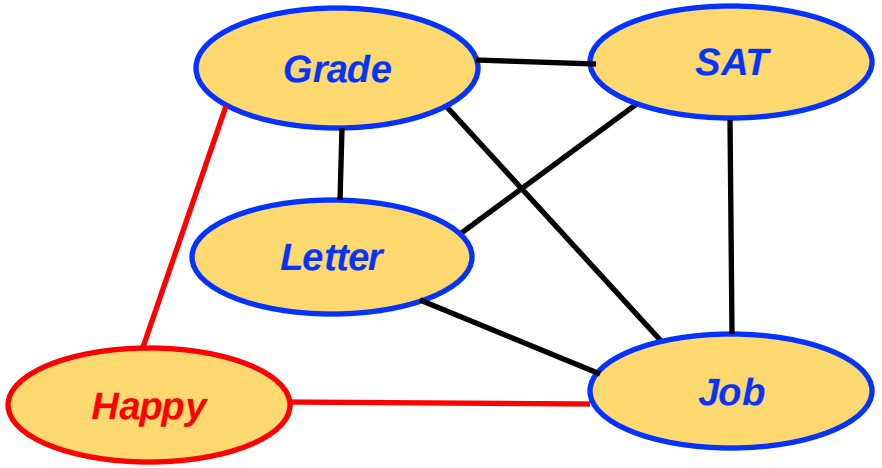
$$\phi(E, G, S) = \mathcal{O}(K^3)$$

Variable Elimination

Elimination order D, E, H, G, S, L

Worst-case Complexity:

$\mathcal{O}(K^3)$



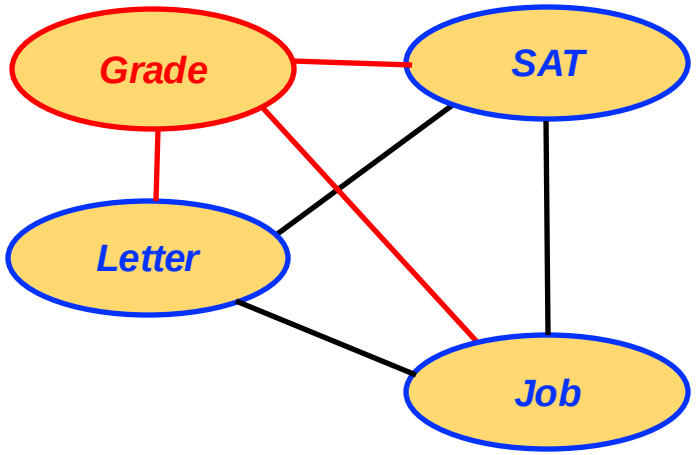
$$\phi(H, G, J) = \mathcal{O}(K^3)$$

Variable Elimination

Elimination order D, E, H, G, S, L

Worst-case Complexity:

$\mathcal{O}(K^4)$



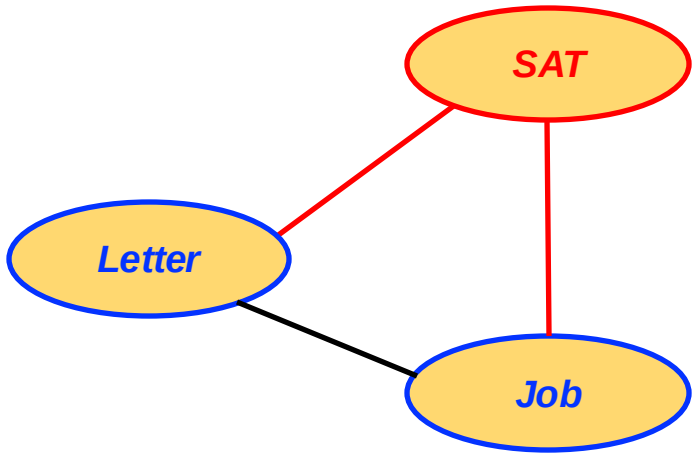
$$\phi(G, S, L, J) = \mathcal{O}(K^4)$$

Variable Elimination

Elimination order D, E, H, G, S, L

Worst-case Complexity:

$\mathcal{O}(K^4)$



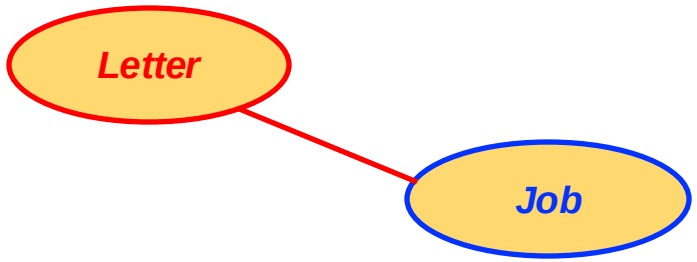
$$\phi(S, L, J) = \mathcal{O}(K^3)$$

Variable Elimination

Elimination order D, E, H, G, S, L

Worst-case Complexity:

$\mathcal{O}(K^4)$



$$\phi(L, J) = \mathcal{O}(K^2)$$

Variable Elimination

Elimination order D, E, H, G, S, L

Worst-case Complexity:

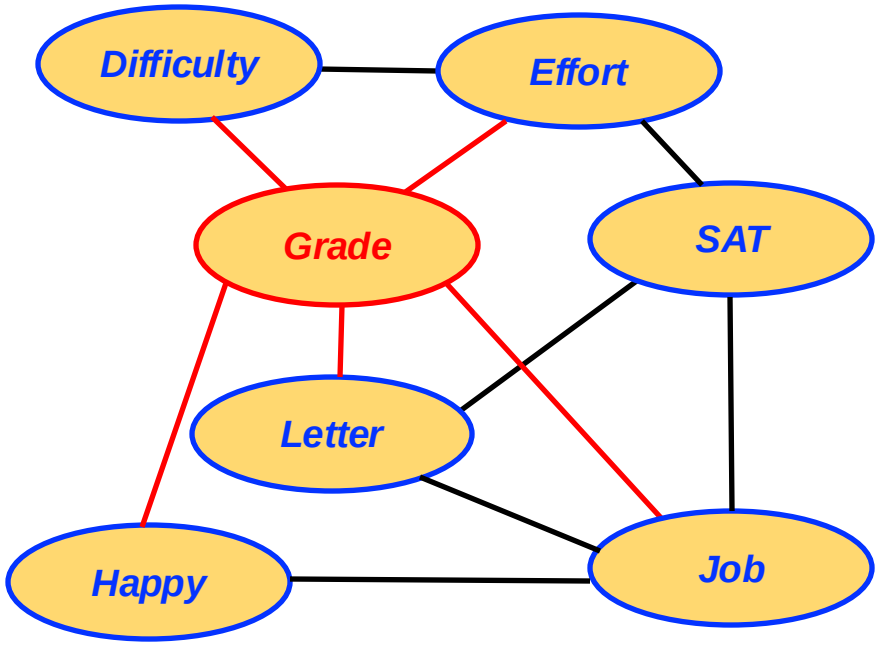
$$\mathcal{O}(K^4)$$

What if we choose a different elimination order?

$$\phi(L, J) = \mathcal{O}(K^2)$$

Computational Complexity

Eliminate G first…



Add fill-in edges to connect all neighbors

Complexity depends on elimination order…

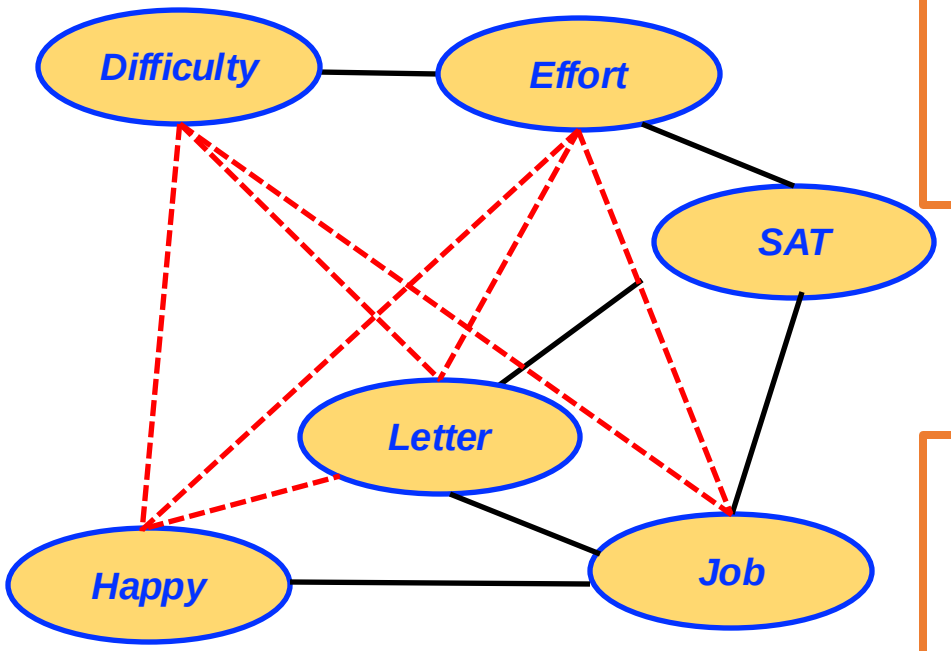
For N variables worst case is:

$$\mathcal{O}(K^N)$$

$$\phi(G, D, E, L, H, J) = \mathcal{O}(K^6)$$

Computational Complexity

Eliminate G first…



Complexity depends on elimination order…

Worst-case Complexity:

$\mathcal{O}(K^6)$

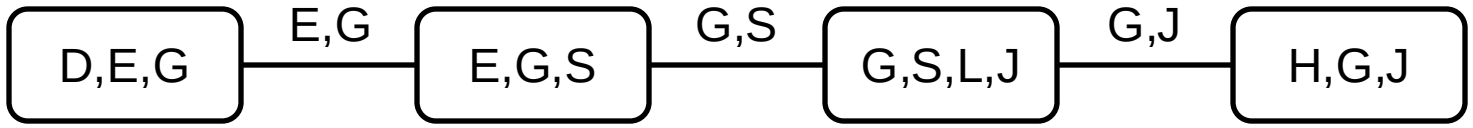
For N variables worst case is:

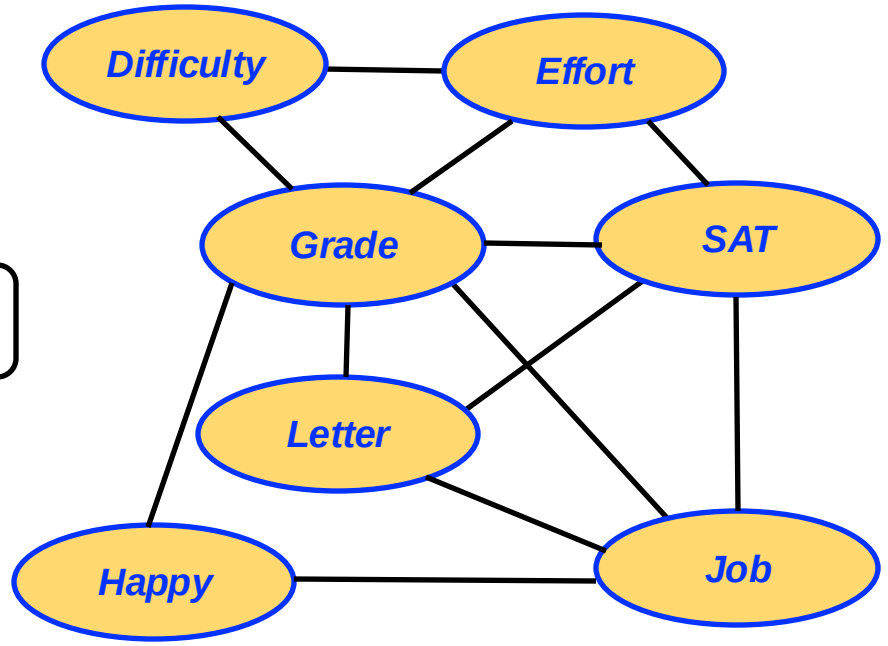
$\mathcal{O}(K^N)$

$$\phi(G, D, E, L, H, J) = \mathcal{O}(K^6)$$

Computational Complexity

Clique Tree





Elimination order $\prec$ induces graph with maximal cliques $\mathcal{C}(\prec)$ and *width:*

$$w(\prec) = \max_{c \in \mathcal{C}(\prec)} |c| - 1$$

- Complexity of variable elimination is $\mathcal{O}(K^{w(\prec)+1})$
- Lowest complexity given by the *treewidth:*

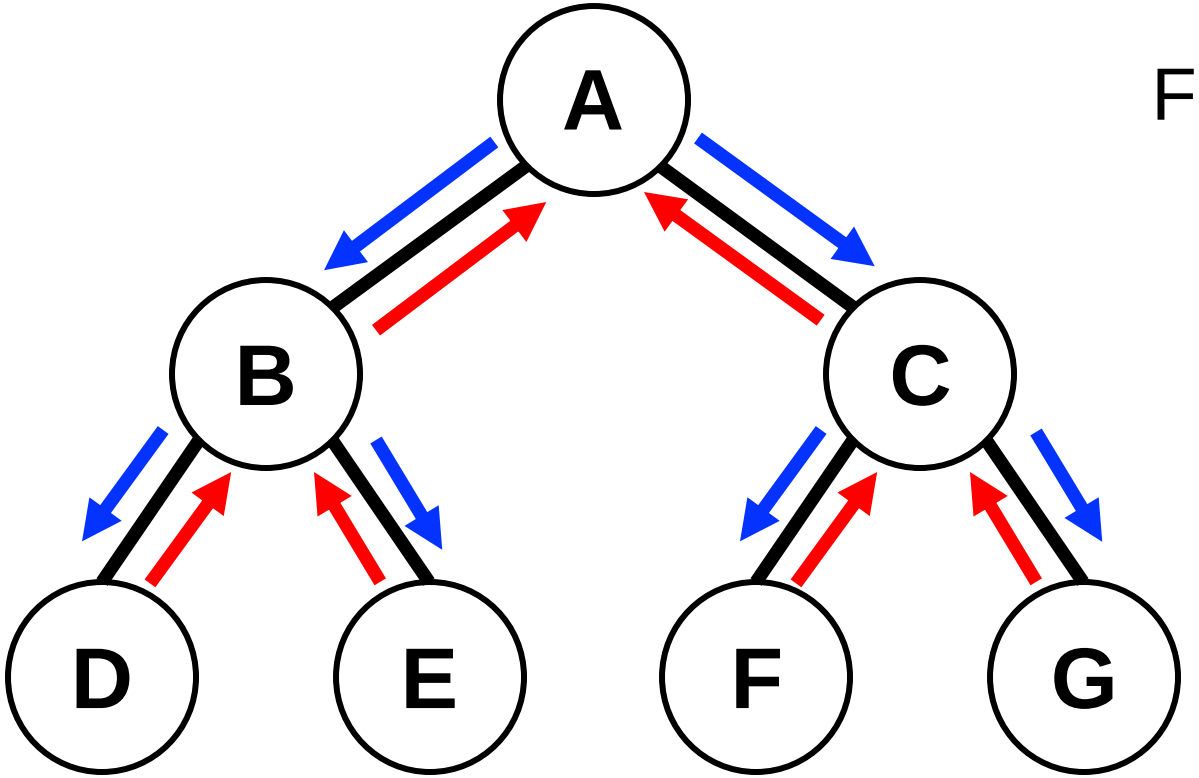
$$w^* = \min_{\prec} \max_{c \in \mathcal{C}(\prec)} |c| - 1$$

It is NP-hard to compute treewidth, and therefore an optimal elimination order (of course…)

Variable Elimination Summary

- Variable elimination allows computation of marginals / conditionals
- Algorithm is valid for **any graphical model**
- Suffices to show variable elimination for MRFs, since Bayes nets → MRFs by *moralization*
- Worst-case complexity is dependent on elimination order, and is **exponential** in number of variables
- Optimal ordering = treewidth, is NP-hard to compute

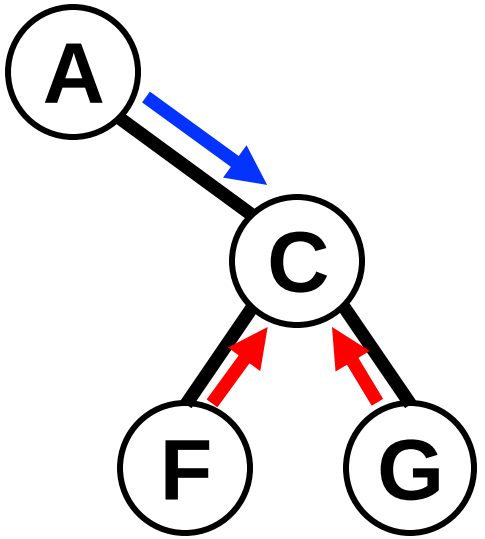
Sum-Product Belief Propagation



Pass messages from leaves-to-root, then root-to-leaves

Forward-Backward extends to *any tree-structured pairwise MRF*

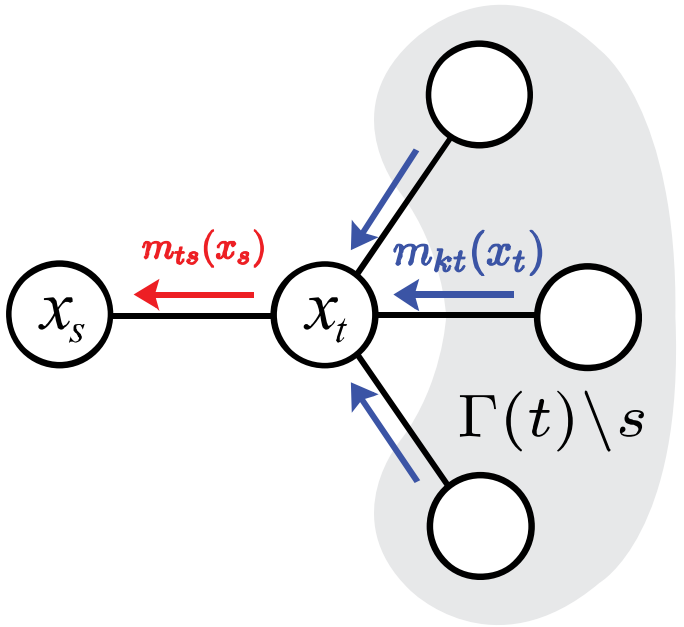
Marginal given by *incoming* messages (e.g. node C):

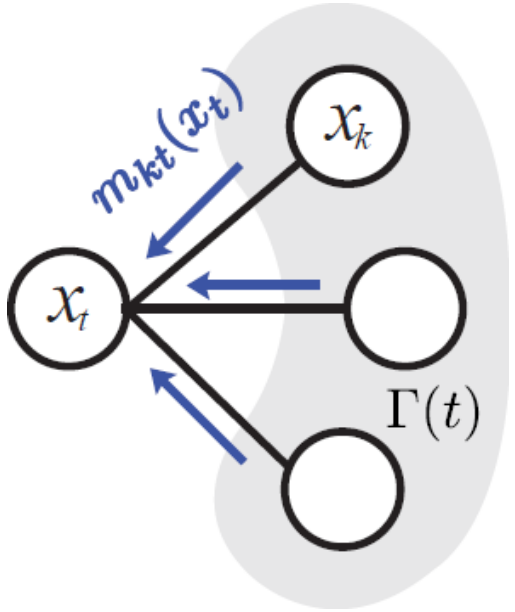


$$p(C) \propto \psi(C) m_A(C) m_F(C) m_G(C)$$

Pairwise MRF Sum-Product Belief Propagation

Message updates depend only on Markov blanket…



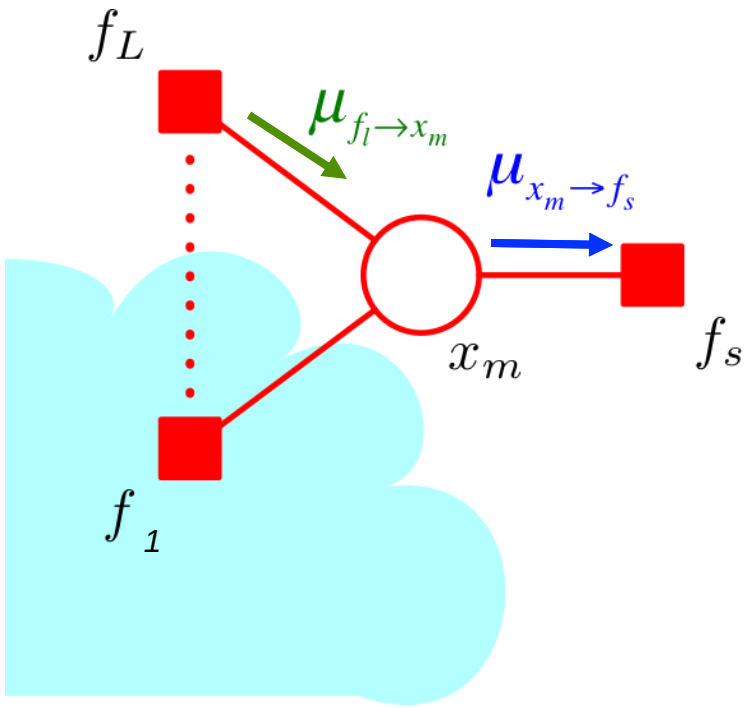


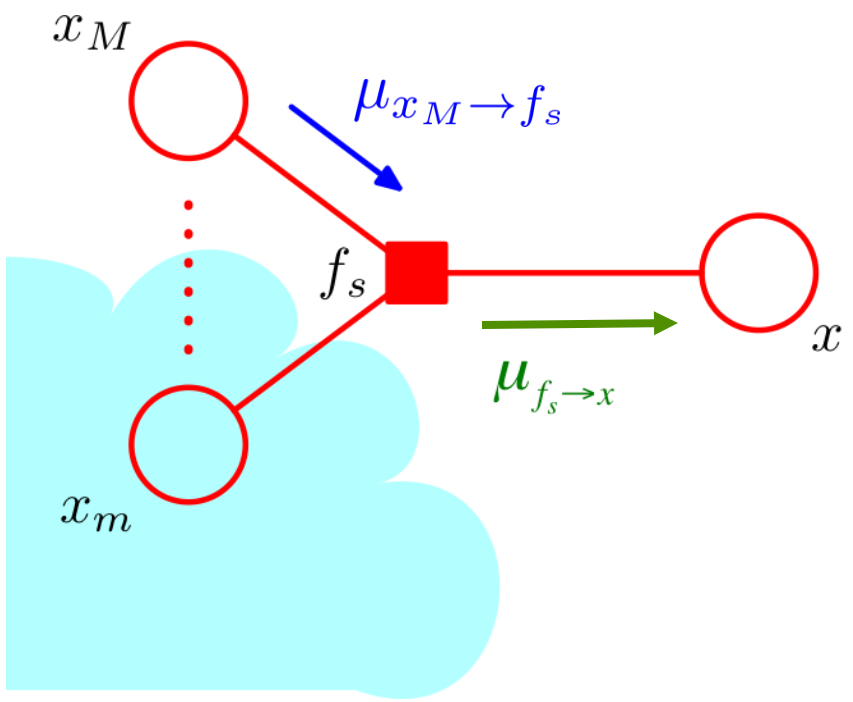
Message $m_{ts}(x_s) = \sum_{x_t} \psi_{st}(x_s, x_t)\psi_t(x_t) \prod_{k\in\Gamma(t)\setminus s} m_{kt}(x_t)$

Marginal $p(x_t) \propto \psi_t(x_t) \prod_{k\in\Gamma(t)} m_{kt}(x_t)$

Messages involve a **sum** over **products**, hence the name "sum-product algorithm"

Factor Graph Sum-Product Belief Propagation





Variable node x_m gathers messages, $\mu_{f_l \to x_m}$, and sends

$$\mu_{x_m \to f_s}(x_m) = \prod_{l \ni f_l \in n(x_m) \setminus f_s} \mu_{f_l \to x_m}(x_m)$$

Factor f_s gathers messages $\mu_{x_m \to f_s}(x_m)$, and sends

$$\mu_{f_s \to x}(x) = \sum_{x_1} \sum_{x_2} \cdots \sum_{x_M} f_s(x, x_1, x_2, \ldots, x_M) \prod_{m \in ne(f_s) \setminus x} \mu_{x_m \to f_s}(x_m)$$

Marginal is product of incoming factor-to-variable messages:

$$p(x_m) \propto \prod_{f_l \in ne(x_m)} \mu_{f_l \to x_m}(x_m)$$

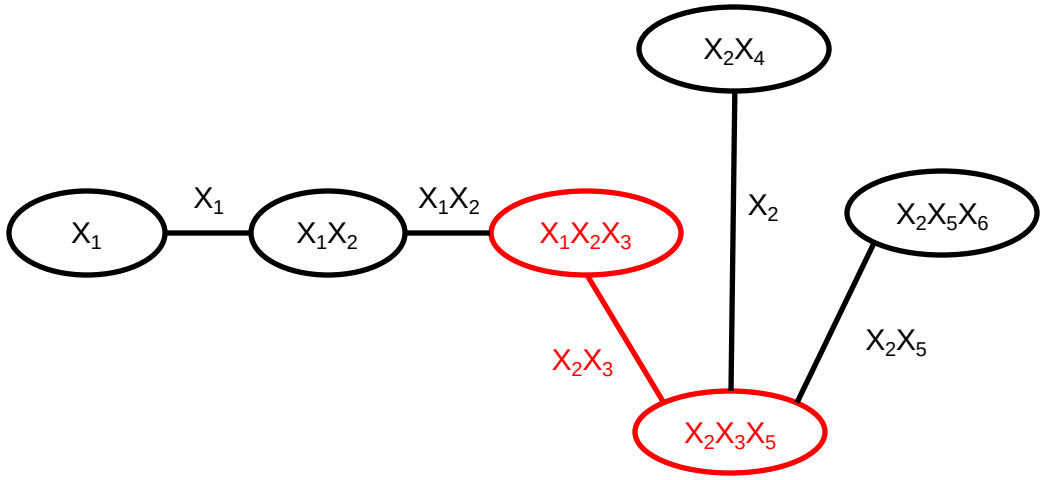
Marginal Inference Algorithms

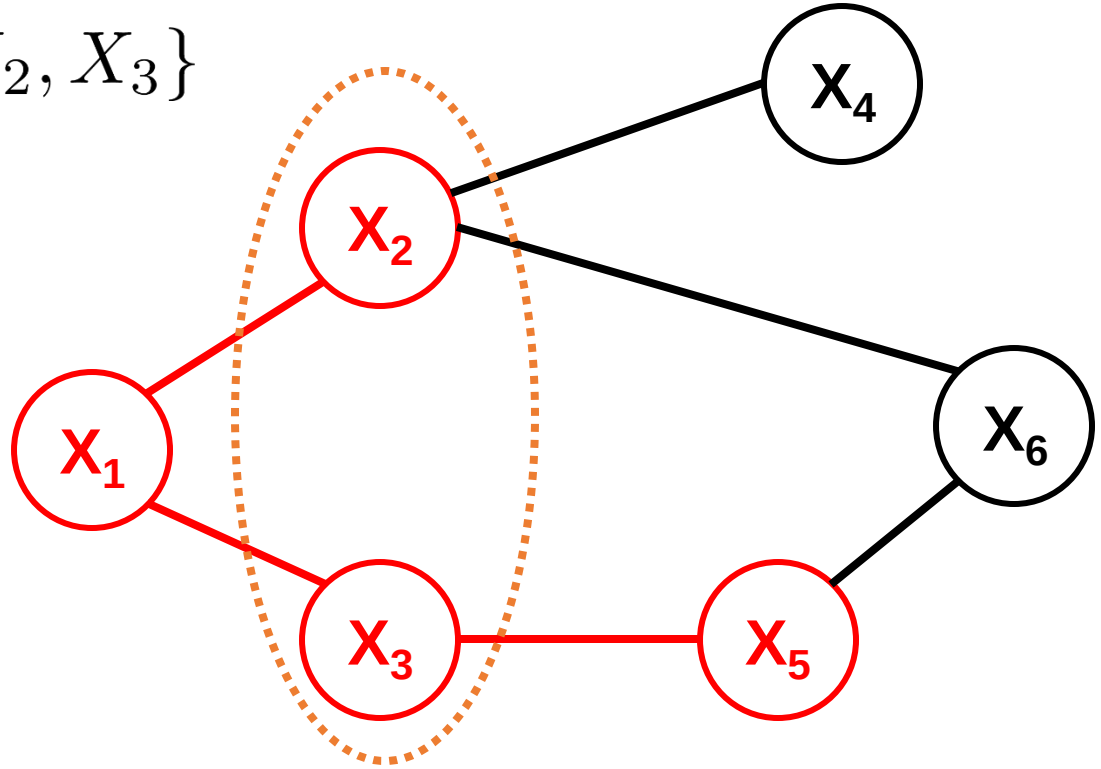
	One Marginal	***All Marginals***
Tree	Elimination applied to leaves of tree	Belief Propagation (BP) or sum-product algorithm
Graph	Variable Elimination	Junction Tree Algorithm BP on a junction tree (special clique tree)

Junction Tree

Clique tree edges are separator sets in original MRF…so clique tree encodes conditional independencies

$$X_1 \perp X_5 \mid \{X_2, X_3\}$$



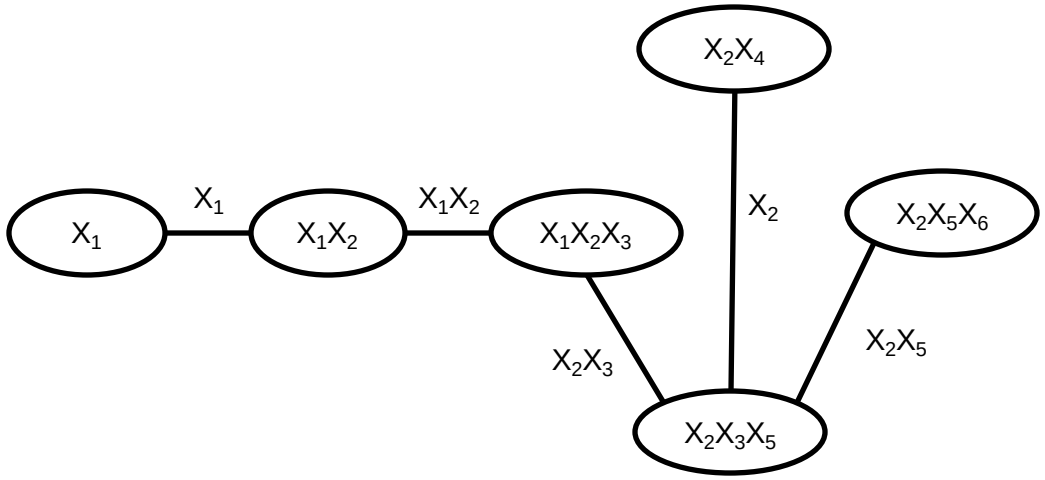


Theorem A clique tree resulting from variable elimination **satisfies the running intersection property** and is thus **a junction tree**

Junction Tree

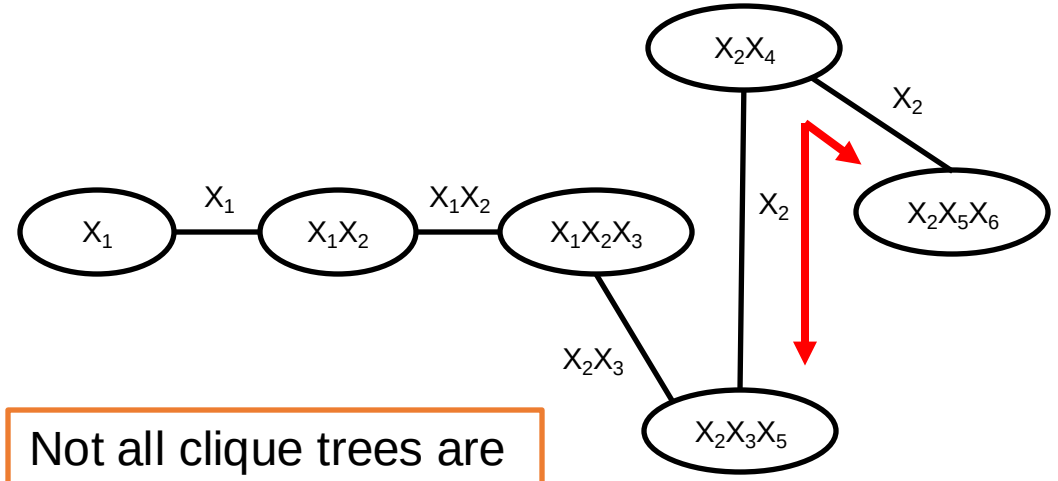
Definition (Running intersection) For any pair of clique nodes V,W all cliques on the *unique path* between V and W contain shared variables

Junction Tree



Not A Junction Tree

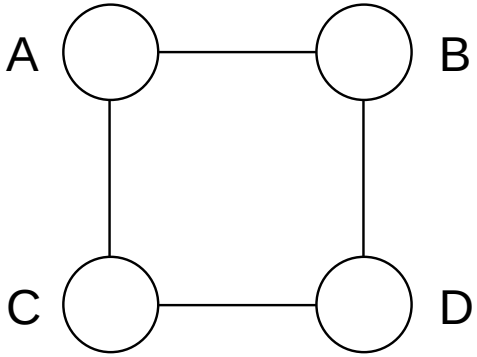
$$\{X_2, X_3, X_5\} \cap \{X_2, X_5, X_6\} = \{X_2, X_5\}$$

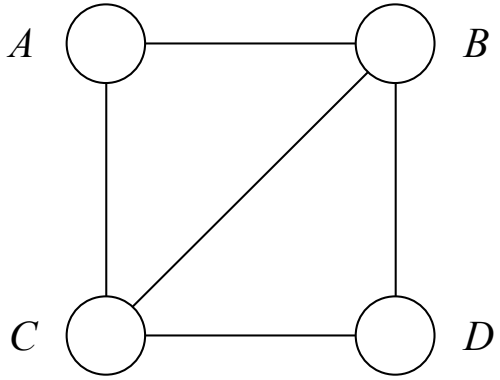


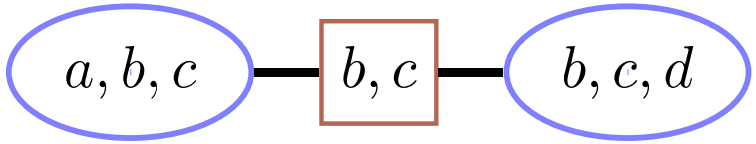
Not all clique trees are junction trees

Theorem A clique tree resulting from variable elimination **satisfies the running intersection property** and is thus **a junction tree**

Junction Trees and Triangulation







- A *chord* is an edge connecting two non-adjacent nodes in some *cycle*
- A cycle is *chordless* if it contains no chords
- A graph is *triangulated (chordal)* if it contains no chordless cycles of length 4 or more

Theorem: The maximal cliques of a graph have a corresponding junction tree *if and only if* that undirected graph is triangulated

Lemma: *For a non-complete triangulated graph with at least 3 nodes, there is a decomposition of the nodes into disjoint sets A, B, S such that S separates A from B, and S is complete.*

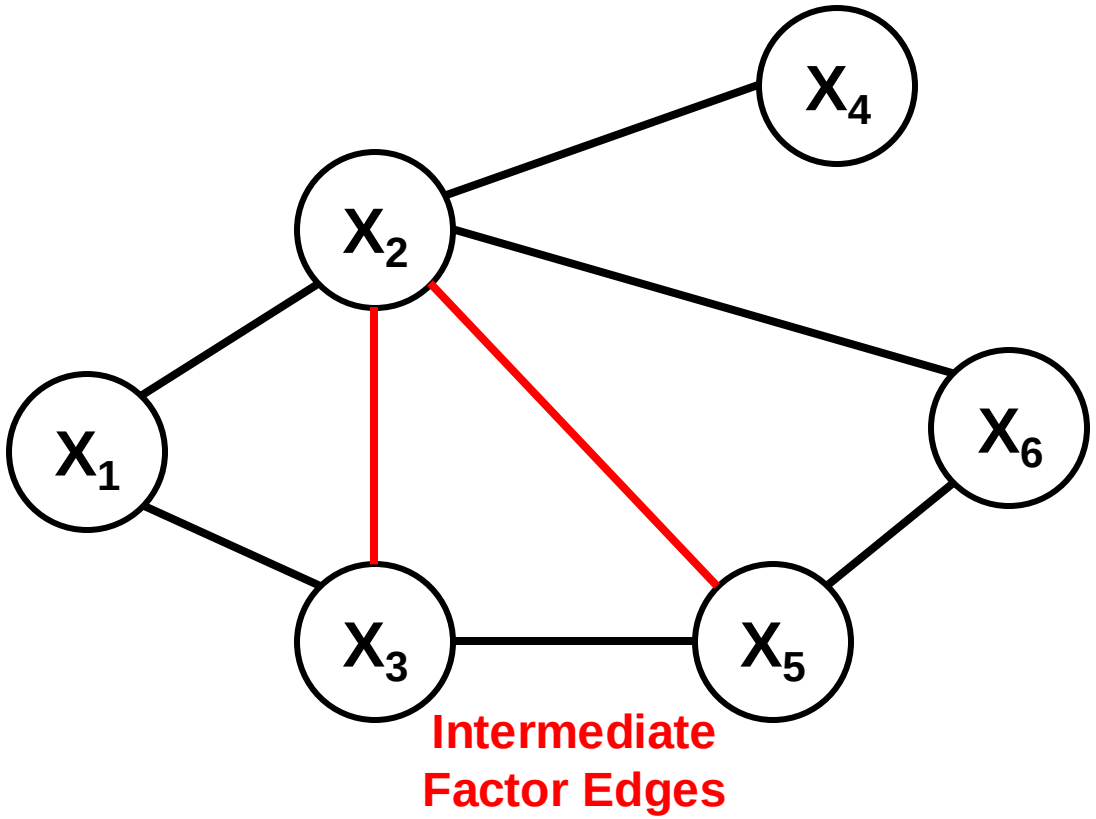
- Key induction argument in constructing junction tree from triangulation
- Implies existence of *elimination ordering which introduces no new edges*

Induced Graph

Recall the **induced graph** is the union over intermediate graphs from running variable elimination

The induced graph **is chordal** thus:

- Maximal cliques of the induced graph form a junction tree
- It admits an elimination ordering that introduces *no new edges*



Logic of junction tree algorithm:

1. Triangulate the graph
   a. Implies a junction tree
   b. Induces an elimination order
2. Run sum-product BP on junction tree to compute **all clique marginals**

Loopy Belief Propagation (sum-product)

Initialize Messages

Constant: $m_{st}^0(x_t) = \text{const.}$

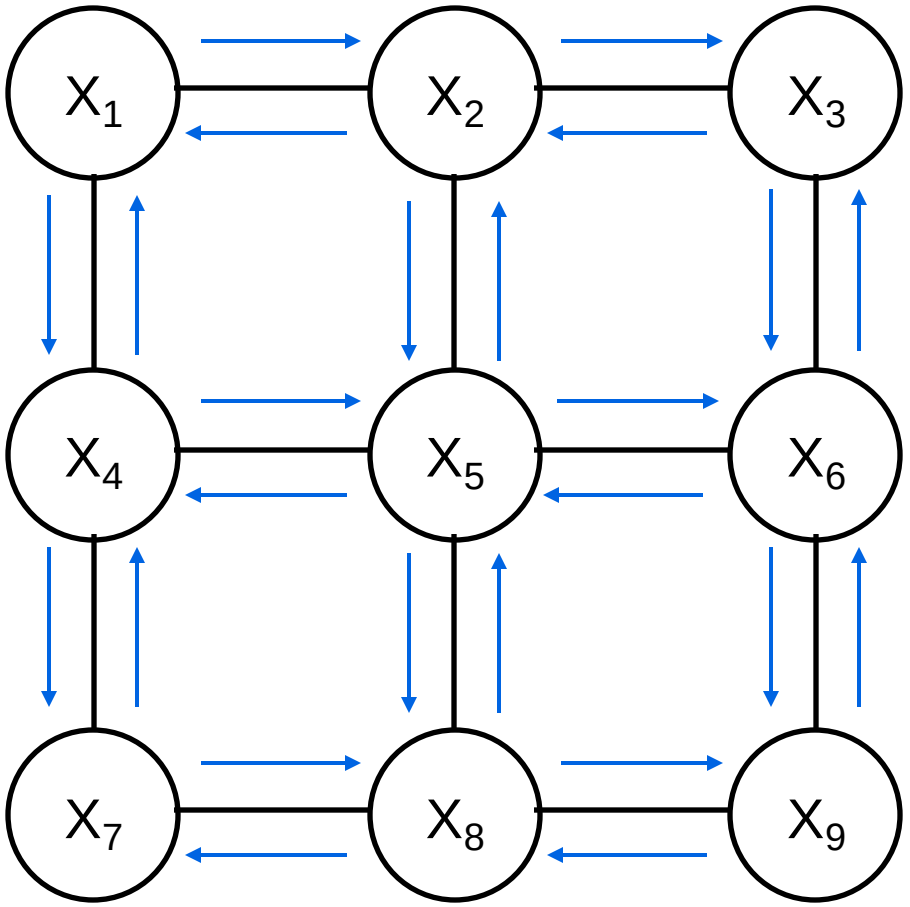
Random: $m_{st}^0(x_t) \sim U([0,1])$

Parallel (Synchronous) Updates

At iteration i update *all messages in parallel* using current messages m^{i-1} from previous iteration:

$$m_{st}^i(x_t) = \sum_{x_s} \psi_{st}(x_s, x_t) \prod_{k \in \Gamma(s) \setminus t} m_{ks}^{i-1}(x_s)$$

- Store, both, the *previous* messages (from iteration *i-1*) and *current* messages (from iteration *i*)
- Many convergence results assume parallel updates



Loopy Belief Propagation (sum-product)

Initialize Messages

Constant: $m_{st}^0(x_t) = \text{const.}$

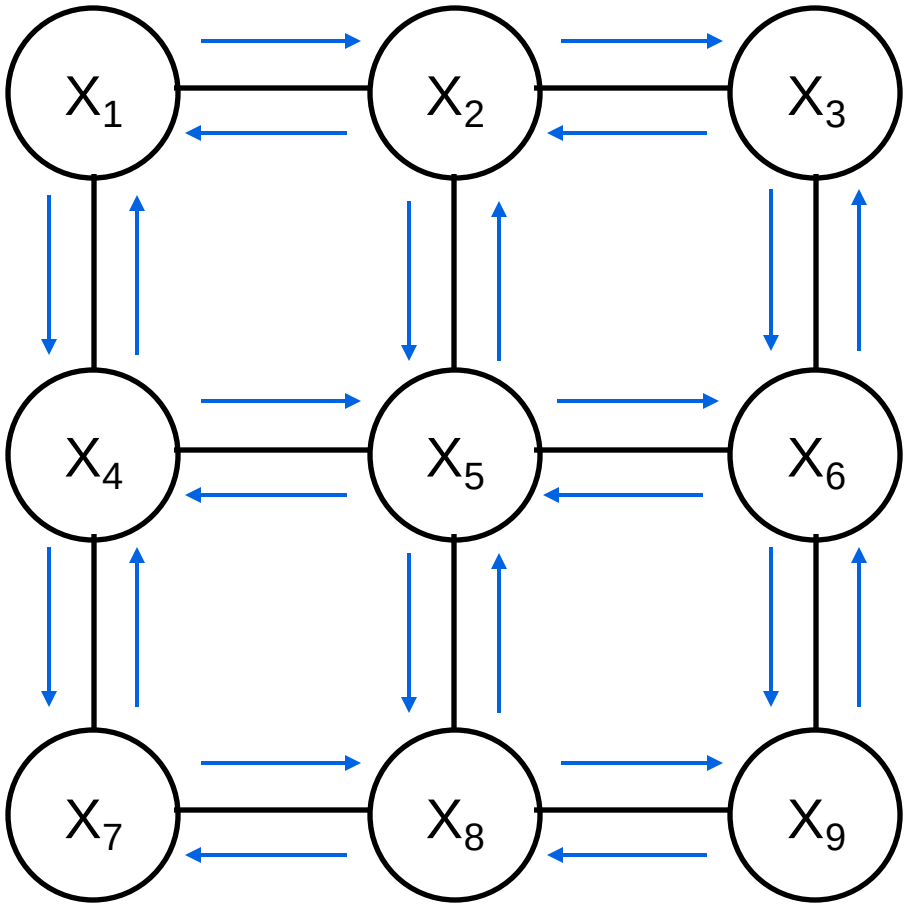
Random: $m_{st}^0(x_t) \sim U([0,1])$

Asynchronous (Sequential) Updates

Choose an ordering of nodes and update using the latest available messages:

$$m_{st}(x_t) = \sum_{x_s} \psi_{st}(x_s, x_t) \prod_{k \in \Gamma(s) \setminus t} m_{ks}(x_s)$$

- Simplifies updates since only need to keep track of one copy of messages
- Makes parallel processing trickier



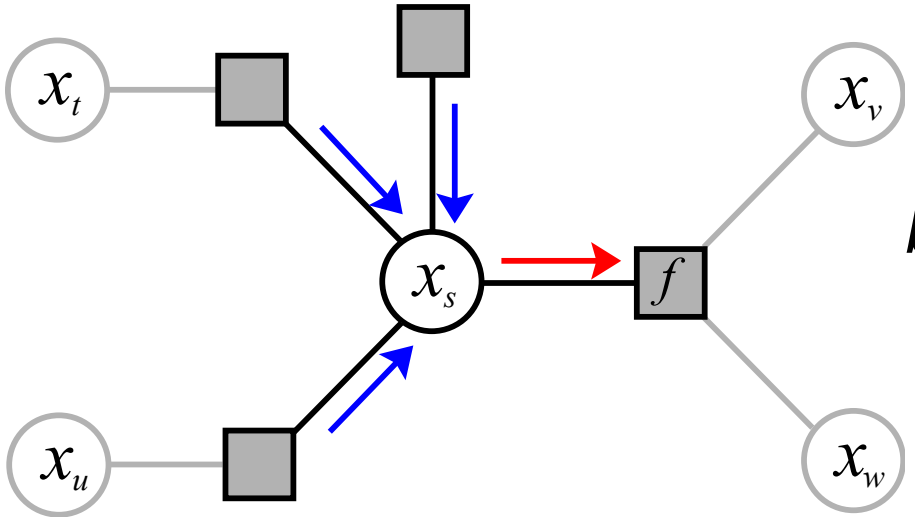
Pseudocode from Murphy's Textbook

Algorithm 22.1: Loopy belief propagation for a pairwise MRF

Input: node potentials $\psi_s(x_s)$, edge potentials $\psi_{st}(x_s, x_t)$;
Initialize messages $m_{s \to t}(x_t) = 1$ for all edges $s - t$;
Initialize beliefs $\text{bel}_s(x_s) = 1$ for all nodes s;
repeat
    Send message on each edge
    $m_{s \to t}(x_t) = \sum_{x_s} \left(\psi_s(x_s) \psi_{st}(x_s, x_t) \prod_{u \in \text{nbr}_s \setminus t} m_{u \to s}(x_s) \right)$;
    Update belief of each node $\text{bel}_s(x_s) \propto \psi_s(x_s) \prod_{t \in \text{nbr}_s} m_{t \to s}(x_s)$;
until *beliefs don't change significantly*;
Return marginal beliefs $\text{bel}_s(x_s)$;

Loopy BP on Factor Graphs

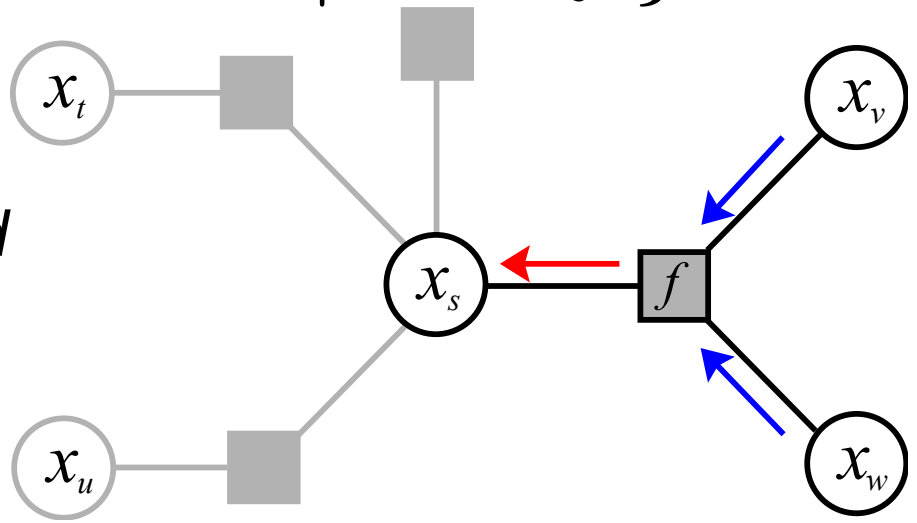
Set of *neighbors* of node s: $\Gamma(s) = \{f \in \mathcal{F} \mid s \in f\}$



Loopy BP:

Message updates can be iteratively computed on graphs with cycles.

But marginals not guaranteed correct!



$$\bar{m}_{sf}(x_s) = \prod_{g \in \Gamma(s) \setminus f} m_{gs}(x_s) \propto \frac{p_s(x_s)}{m_{fs}(x_s)}$$

$$m_{fs}(x_s) = \sum_{x_{f \setminus s}} \psi_f(x_f) \prod_{t \in f \setminus s} \bar{m}_{tf}(x_t)$$

Marginal Distribution of Each Variable:

$$p_s(x_s) \propto \prod_{f \in \Gamma(s)} m_{fs}(x_s)$$

Marginal Distribution of Each Factor:

Clique of variables linked by factor.

$$p_f(x_f) \propto \psi_f(x_f) \prod_{s \in f} \bar{m}_{sf}(x_s)$$

Message Passing Inference Summary

- Brute-force enumeration exponential regardless of graph
- Sum-Product BP
  - Exact inference in tree-structure graphs in $O(TK^2)$ time for T nodes, each taking K states
  - Reduces to Forward-Backward in HMMs
  - Same for Max-Product BP (reduces to Viterbi in HMMs)
- Variable elimination
  - Exact marginals in general graphs
  - Worst-case complexity exponential in size of largest clique
  - Need to rerun from scratch for each marginal
  - Complexity dependent on elimination order (NP-hard to optimize)

Message Passing Inference Summary

- Junction Tree Algorithm
  - Exact marginals in general graphs
  - Caches messages to compute all marginals
  - Worst-case complexity exponential in size of largest clique
  - Optimizing Jtree is NP-hard (corresponds to finding treewidth)

- Loopy BP
  - BP updates only depend on tree-structured Markov blanket
  - **Approximate** inference in loopy graphs
  - No guarantees, but works well empirically in many instances
  - Some techniques to improve convergence
    - Message damping
    - Asynchronous message update schedules

Topics

- Probability and Statistics
- Probabilistic Graphical Models
- Message Passing Inference
- Parameter Learning
- Monte Carlo Methods

Maximum Likelihood Estimation

$$\theta^{\mathrm{MLE}} = \arg\max_{\theta} p(\mathcal{Y} \mid \theta) = \arg\max_{\theta} \log p(\mathcal{Y} \mid \theta)$$

If concave then just solve for zero-gradient solution,

$$\mathcal{L}(\theta) \equiv \log p(\mathcal{Y} \mid \theta) \qquad \nabla_\theta \mathcal{L}(\theta^{\mathrm{MLE}}) = 0$$

Log-Likelihood Function doesn't change argmax since log is monotonic

Logarithm serves a couple of practical purposes:

1) Simplifies derivatives for conditionally independent data

$$\nabla_\theta \mathcal{L}(\theta) = \sum_{i=1}^{N} \nabla_\theta \log p(y_i \mid \theta)$$

2) Avoids numerical under/overflow

MLE of Gaussian Mean

Assume data are i.i.d. univariate Gaussian,

$$p(\mathcal{Y} \mid \theta) = \prod_{i=1}^{N} \mathcal{N}(y_i \mid \theta, \sigma^2)$$

Variance is known

Log-likelihood function:

$$\mathcal{L}(\theta) = \sum_{i=1}^{N} \log \left(\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2}(y_i - \theta)^2 \sigma^{-2} \right) \right)$$

Constant doesn't depend on mean

$$= \text{const.} - \frac{1}{2} \sum_{i=1}^{N} \left((y_i - \theta)^2 \sigma^{-2} \right)$$

MLE doesn't change when we:
1) Drop constant terms (in θ)
2) Minimize negative log-likelihood

MLE estimate is *least squares estimator*:

$$\theta^{\text{MLE}} = -\frac{1}{2\sigma^2} \arg\max_{\theta} \sum_{i=1}^{N} (y_i - \theta)^2 = \arg\min_{\theta} \sum_{i=1}^{N} (y_i - \theta)^2$$

Maximum A Posteriori (MAP) Estimation

Recall the MAP estimator maximizes posterior probability,

$$\theta^{\mathrm{MAP}} = \arg\max_{\theta} p(\theta \mid \mathcal{Y})$$

$$= \arg\max_{\theta} p(\theta, \mathcal{Y}) \quad \textbf{(Bayes' rule)}$$

$$= \arg\max_{\theta} p(\mathcal{Y} \mid \theta) p(\theta) \quad \textbf{(Probability Chain Rule)}$$

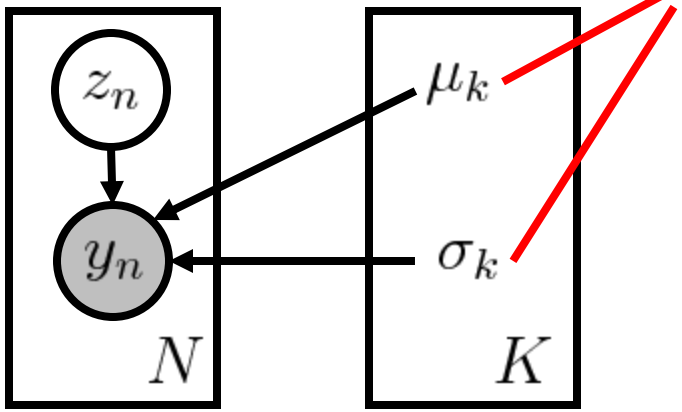
$$= \arg\max_{\theta} \log p(\mathcal{Y} \mid \theta) + \log p(\theta) \quad \textbf{(Monotonicity of Logarithm)}$$

Prior serves as regularizer in regularized MLE:

$$\theta^{\mathrm{MLE}} = \arg\max_{\theta} \mathcal{L}(\theta) - \lambda R(\theta)$$

Marginal Likelihood Calculation

Recall the Gaussian Mixture Model…

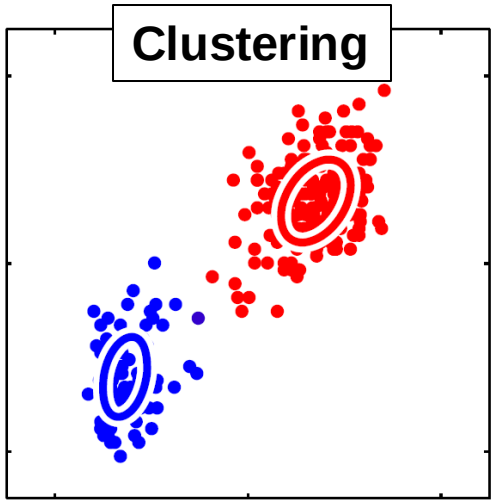


$$\theta = \{\mu_1, \sigma_1, \ldots, \mu_K, \sigma_K\}$$

Marginal Likelihood (likelihood function):

$$p(\mathcal{Y} \mid \theta) = \underbrace{\sum_{z_1} \cdots \sum_{z_N}} p(z_1, \ldots, z_N, \mathcal{Y} \mid \theta)$$

Sum over all possible K^N assignments, which we cannot compute



Motivation Approximate MLE / MAP when we cannot compute the marginal likelihood in closed-form

Expectation Maximization

Complete Data Log-Likelihood

$$\max_{\theta} \log p(\mathcal{Y} \mid \theta) \geq \max_{q,\theta} \mathbf{E}_q \left[\log \frac{p(z, \mathcal{Y} \mid \theta)}{q(z)} \right] \equiv \mathcal{L}(q, \theta)$$

Initialize Parameters: $\theta^{(0)}$

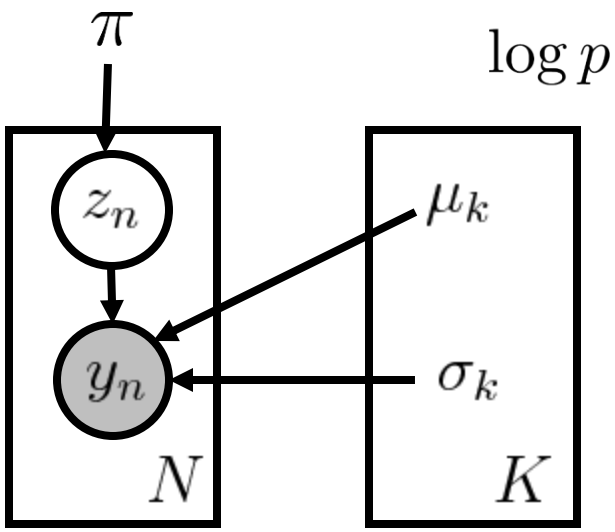
At iteration t do:

E-Step: $q^{(t)}(z) = p(z \mid y, \theta^{(t-1)})$

M-Step: $\theta^{(t)} = \arg\max_{\theta} \mathcal{L}(q^{(t)}, \theta)$

Until convergence

Example: Gaussian Mixture Model



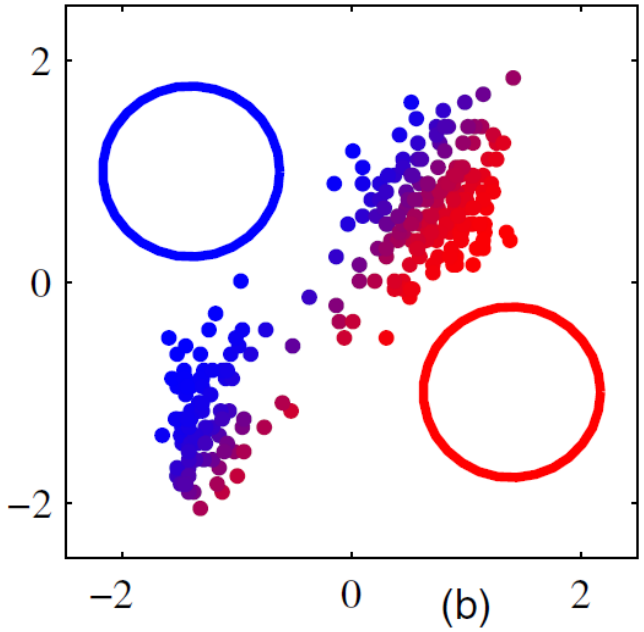
$$\log p(\mathcal{Y} \mid \pi, \mu, \Sigma) \geq \sum_{n=1}^{N} \sum_{k=1}^{K} q(z_n = k) \log \{\pi_k \mathcal{N}(y_n \mid \mu_k, \Sigma_k)\} = \mathcal{L}(q, \theta)$$

E-Step: $q^{\text{new}} = \arg\max_q \mathcal{L}(q, \theta^{\text{old}})$

$$q^{\text{new}}(z_n = k) = p(z_n = k \mid \mathcal{Y}, \mu^{\text{old}}, \Sigma^{\text{old}}, \pi^{\text{old}})$$

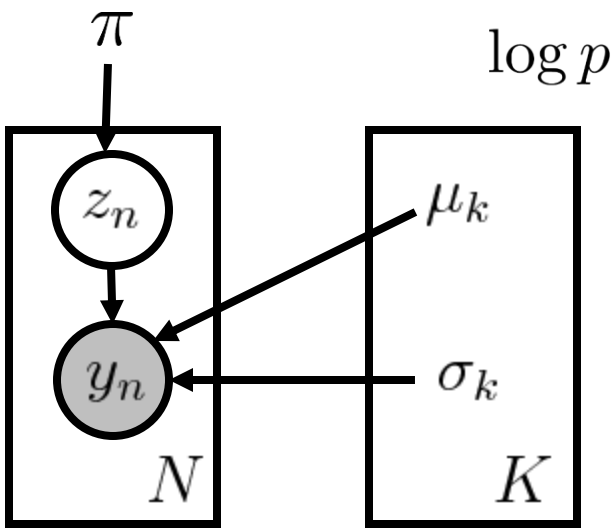
$$= \frac{p(z_n = k, \mathcal{Y} \mid \mu^{\text{old}}, \Sigma^{\text{old}}, \pi^{\text{old}})}{\sum_{j=1}^{K} p(z_n = j, \mathcal{Y} \mid \mu^{\text{old}}, \Sigma^{\text{old}}, \pi^{\text{old}})}$$

$$= \frac{\pi_k \mathcal{N}(y_n \mid \mu_k^{\text{old}}, \Sigma_k^{\text{old}})}{\sum_{j=1}^{K} \pi_j \mathcal{N}(y_n \mid \mu_j^{\text{old}}, \Sigma_j^{\text{old}})}$$



Commonly refer to $q(z_n)$ as *responsibility*

Example: Gaussian Mixture Model



$$\log p(\mathcal{Y} \mid \pi, \mu, \Sigma) \geq \sum_{n=1}^{N} \sum_{k=1}^{K} q(z_n = k) \log \{\pi_k \mathcal{N}(y_n \mid \mu_k, \Sigma_k)\} = \mathcal{L}(q, \theta)$$

M-Step: $\theta^{\text{new}} = \arg\max_{\theta} \mathcal{L}(q^{\text{new}}, \theta)$

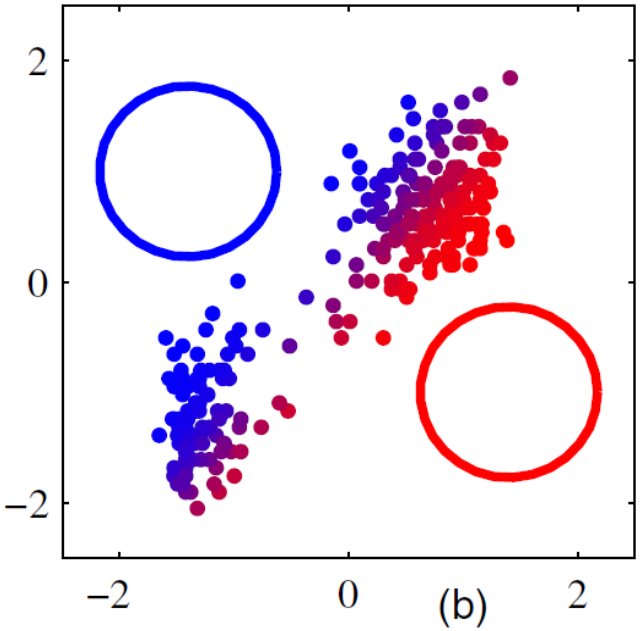
Start with mean parameter μ_k,

$$0 = \nabla_{\mu_k} \mathcal{L}(q^{\text{new}}, \theta)$$

$$0 = \sum_{n=1}^{N} \nabla_{\mu_k} \mathbf{E}_{z_n \sim q^{\text{new}}} [\log \mathcal{N}(y_n \mid \mu_{z_n}, \Sigma_{z_n})]$$

$$0 = -\sum_{n=1}^{N} q^{\text{new}}(z_n = k) \Sigma_k (y_n - \mu_k)$$

$$\mu_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} q^{\text{new}}(z_n = k) y_n \quad \text{where} \quad N_k = \sum_{n=1}^{N} q(z_n = k)$$



EM Lower Bound

$$\mathbf{E}_q\left[\log \frac{p(z, y \mid \theta)}{q(z)}\right] = \mathbf{E}_q\left[\log \frac{p(z, y \mid \theta)}{q(z)} \frac{p(y \mid \theta)}{p(y \mid \theta)}\right]$$

(Multiply by 1)

$$= \log p(y \mid \theta) - \mathrm{KL}(q(z) \| p(z \mid y, \theta))$$

(Definition of KL)

Bound gap is the Kullback-Leibler divergence KL(q||p),

$$\mathrm{KL}(q(z) \| p(z \mid y, \theta)) = \sum_z q(z) \log \frac{q(z)}{p(z \mid y, \theta)}$$

- Similar to a “distance” between q and p

$$\mathrm{KL}(q \mid\mid p) \geq 0 \text{ and } \mathrm{KL}(q \mid\mid p) = 0 \text{ if and only if } q = p$$

- This is why solution to E-step is $q(z) = p(z \mid y, \theta)$

Properties of Expectation Maximization Algorithm

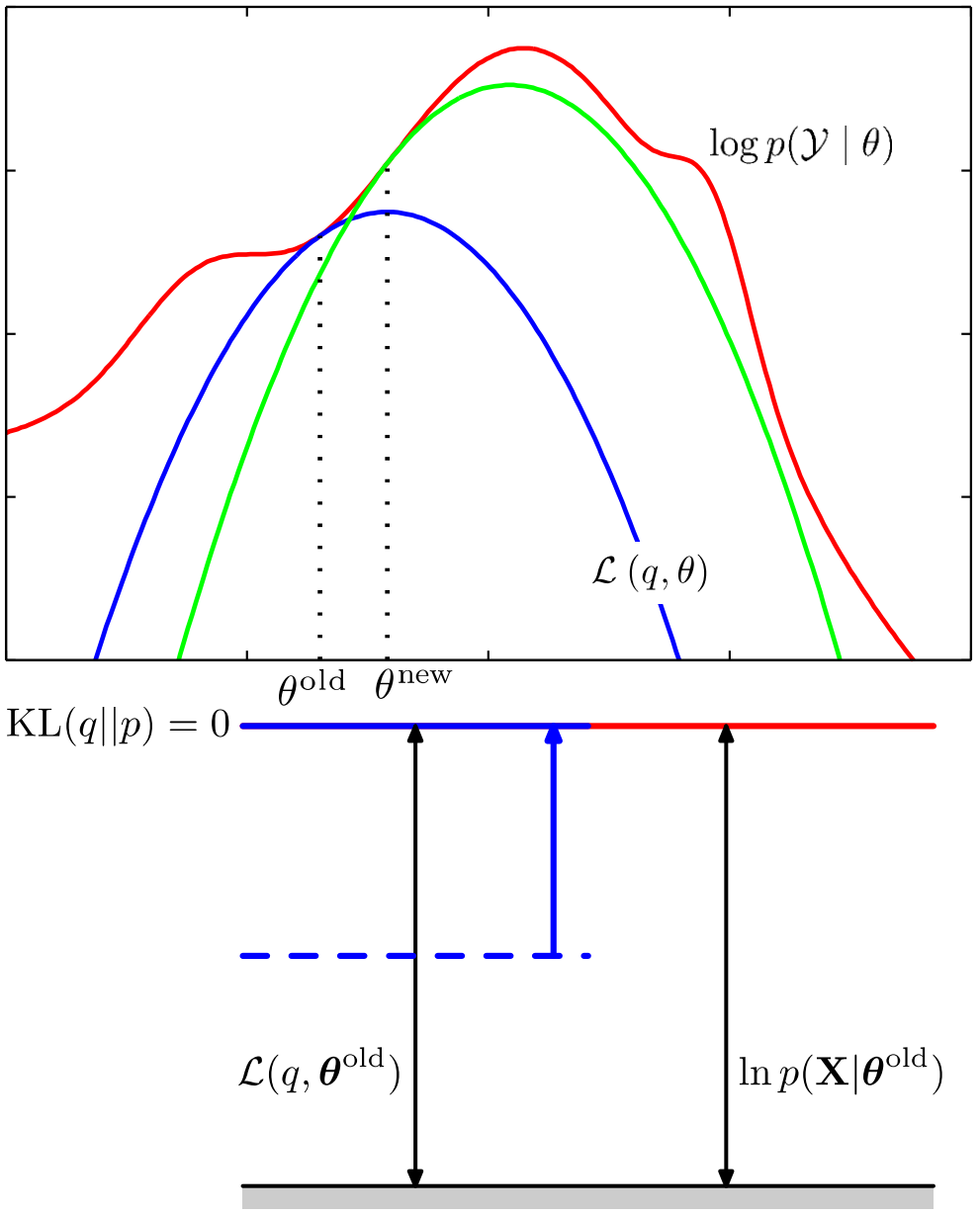
Sequence of bounds is monotonic,

$$\mathcal{L}(q^{(1)}, \theta^{(1)}) \leq \mathcal{L}(q^{(2)}, \theta^{(2)}) \leq \ldots \leq \mathcal{L}(q^{(T)}, \theta^{(T)})$$

Guaranteed to converge
(**Pf.** Monotonic sequence bounded above.)

Converges to a local maximum of the marginal likelihood

After each E-step bound is tight at θ^{old}
so likelihood calculation is exact (for those parameters)



MAP EM

Easily extends to (approximate) MAP estimation,

$$\max_{\theta} \log p(\theta \mid \mathcal{Y}) \geq \max_{q,\theta} \mathbf{E}_q \left[\log \frac{p(z, \mathcal{Y} \mid \theta)}{q(z)} \right] + \log p(\theta) + \text{const.}$$

E-step unchanged / Slightly modifies M-step,

E-Step

$$\begin{aligned} q^{\text{new}} &= \arg\max_{q} \mathcal{L}(q, \theta^{\text{old}}) \\ &= p(z \mid \mathcal{Y}, \theta^{\text{old}}) \end{aligned}$$

M-Step

$$\theta^{\text{new}} = \arg\max_{\theta} \mathcal{L}(q^{\text{new}}, \theta) + \log p(\theta)$$

Properties of both MLE / MAP EM

- Monotonic in $\mathcal{L}(q, \theta)$ or $\mathcal{L}(q, \theta) + \log p(\theta)$ (for MAP)
- Provably converge to local optima (hence approximate estimation)

Learning Summary

Maximum a posteriori (MAP) maximizes posterior probability,

$$\theta^{\mathrm{MAP}} = \arg\max_{\theta} \log p(\theta \mid \mathcal{Y}) = \arg\max_{\theta} \mathcal{L}(\theta) + \log p(\theta)$$

Parameters are *random* quantities with prior $p(\theta)$.

Corresponds to regularized MLE for specific prior/regularizer pair,

$$\hat{\theta} = \arg\max_{\theta} \mathcal{L}(\theta) - \lambda \mathcal{R}(\theta)$$

Gaussian prior=L2, Laplacian prior=L1

Straightforward sequential updating, e.g. Bayesian linear regression

Topics

- Probability and Statistics
- Probabilistic Graphical Models
- Message Passing Inference
- Parameter Learning
- Monte Carlo Methods

Inference (and related) Tasks

- Simulation: $x \sim p(x) = \frac{1}{Z} f(x)$
- Compute expectations: $\mathbb{E}[\phi(x)] = \int p(x)\phi(x)\, dx$
- Optimization: $x^* = \arg\max_x f(x)$
- Compute normalizer / marginal likelihood: $Z = \int f(x)\, dx$

Inference (and related) Tasks

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Monte Carlo Estimation

One reason to sample a distribution is to approximate expected values under that distribution…

Expected value of function $f(x)$ w.r.t. distribution $p(x)$ given by,

$$\mathbb{E}_p[f(x)] = \int p(x)f(x)\,dx \equiv \mu$$

- Doesn't always have a closed-form for arbitrary functions
- Suppose we have iid samples: $\{x_i\}_{i=1}^N \sim p(x)$
- *Monte Carlo* estimate of expected value,

$$\hat{\mu}_N = \frac{1}{N}\sum_{i=1}^{N} f(x_i) \approx \mathbb{E}_p[f(x)]$$

Samples must be independent!

Markov chain Monte Carlo methods

- The approximations of expectation that we have looked at so far have assumed that the samples are independent draws.
- This sounds good, but in high dimensions, we do not know how to get good independent samples from the distribution.
- MCMC methods drop this requirement.
- Basic intuition
  - If you have finally found a region of high probability, stick around for a bit, enjoy yourself, grab some more samples.

Markov chain Monte Carlo methods

- Samples are conditioned on the previous one (this is the Markov chain).
- MCMC is often a good hammer for complex, high dimensional, problems.
- Main downside is that it is not “plug-and-play”
  - Doing well requires taking advantage to the structure of your problem
  - MCMC tends to be expensive (but take heart---there may not be any other solution, and at least your problem is being solved).
  - If there are faster solutions, you can incorporate that (and MCMC becomes a way to improve/select these good guesses).

Metropolis Algorithm

We want samples $z^{(1)}, z^{(2)}, \ldots$.

Again, write $p(z) = \tilde{p}(z)/Z$

Assume that $q\left(z \middle| z^{(prev)}\right)$ can be sampled easily

Also assume that $q(\ \ )$ is symmetric, i.e., $q\left(z_A \middle| z_B\right) = q\left(z_B \middle| z_A\right)$

For example, $q\left(z \middle| z^{(prev)}\right) \sim \mathbb{N}\left(z; z^{(prev)}, \sigma^2\right)$

Metropolis Algorithm

While not_bored

{

Sample $q\left(z \middle| z^{(prev)}\right)$

Accept with probability $A\left(z, z^{(prev)}\right) = \min\left(1, \frac{\tilde{p}(z)}{\tilde{p}\left(z^{(prev)}\right)}\right)$

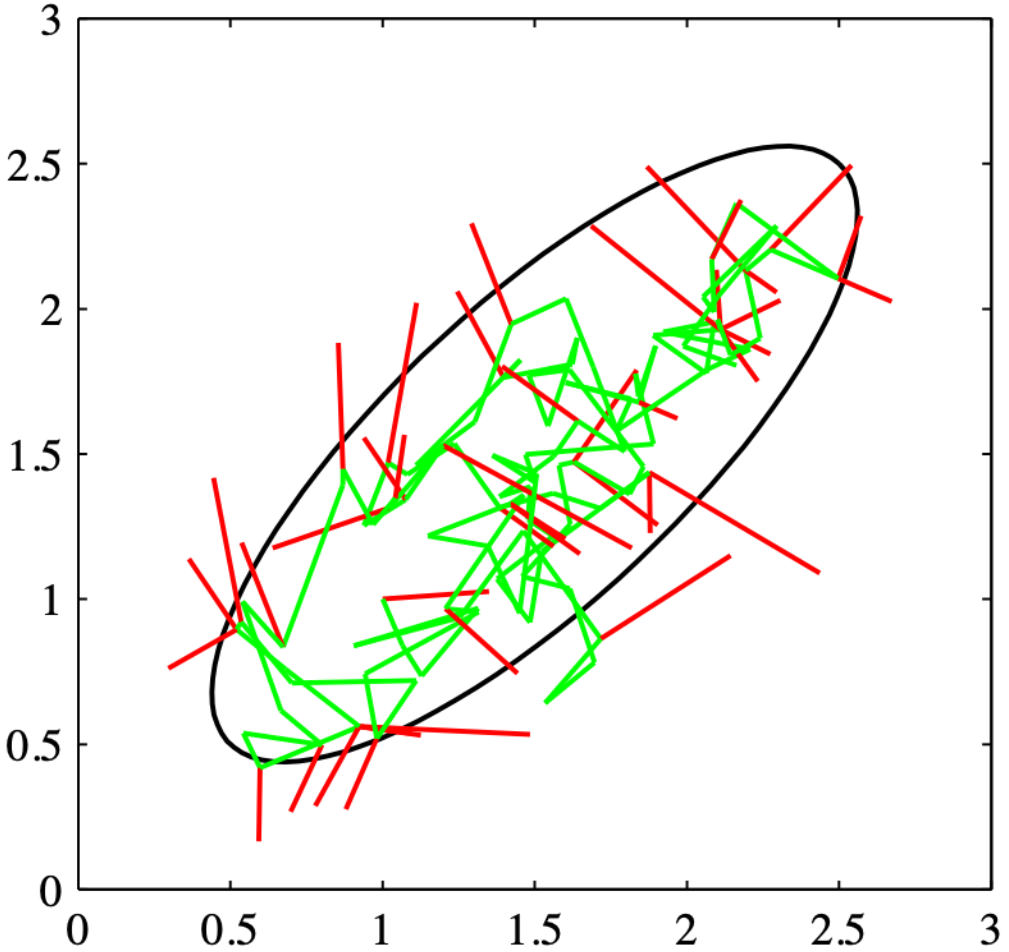
If accept, emit z, otherwise, emit $z^{(prev)}$.

}

Always emit one or the other

If things get better, always accept. If they get worse, sometimes accept.

Metropolis Example



Green follows accepted proposals
Red are rejected moves.

Beyond the Metropolis Method

Metropolis requires the proposal to be symmetric,

$$q(z' \mid z) = q(z \mid z')$$

This often results in a chain that takes a long time to converge to a stationary distribution (long burn in time)

Example The most common proposal (Gaussian),

$$q(z' \mid z) = \mathcal{N}(z' \mid z, \sigma^2 I)$$

exhibits random walk dynamics that are inefficient

Metropolis-Hastings relaxes this symmetry requirement…

Metropolis-Hastings MCMC method

While not_bored

{

Sample $q\left(z \middle| z^{(prev)}\right)$

Accept with probability $A\left(z, z^{(prev)}\right) = \min\left(1, \frac{\tilde{p}(z) q\left(z^{(prev)} \middle| z\right)}{\tilde{p}\left(z^{(prev)}\right) q\left(z \middle| z^{(prev)}\right)}\right)$

If accept, emit z, otherwise, emit $z^{(prev)}$.

}

Does Metropolis-Hastings converge to the target distribution?

- Like Metropolis, but now q() is not necessarily symmetric.

- If Metropolis-Hastings has detailed balance, then it converges to the target distribution under weak conditions.
  - The converse is not true, but generally samplers of interest will have detailed balance

MCMC So Far…

Metropolis Algorithm

- Sample RV from proposal $z \sim q(z \mid z^{(\text{prev})})$
- Proposal must be *symmetric*: $q(z \mid z^{(\text{prev})}) = q(z^{(\text{prev})} \mid z)$
- Accept with probability $\min\left\{1, \widetilde{p}(z) \div \widetilde{p}(z^{(\text{prev})})\right\}$

Metropolis-Hastings Algorithm

- Proposal does not have to be symmetric
- Accept with probability

$$\min\left\{1, \frac{\widetilde{p}(z)q(z^{(\text{prev})} \mid z)}{\widetilde{p}(z^{(\text{prev})})q(z \mid z^{(\text{prev})})}\right\}$$

Both methods require choosing proposal, which can be hard

Gibbs Sampling

Let $p(x)$ be the target distribution on random variables,

$$x_1, x_2, \ldots, x_N$$

Consider the *complete conditional distribution* x_i

$$p(x_i \mid x_{\neg i})$$

where $x_{\neg i} = \{x_1, x_2, \ldots, x_N\} \backslash x_i$ all RVs *except* x_i

Idea Don't sample all RVs from one proposal. Sample each from its corresponding complete conditional,

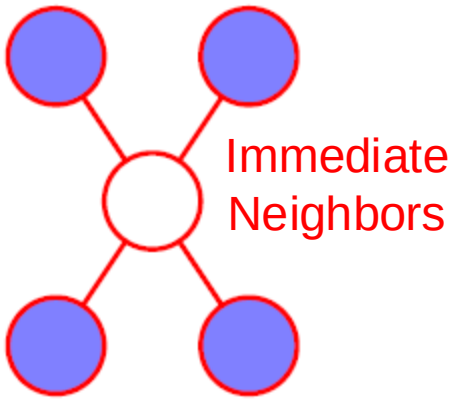
$$q_i(x_i \mid x_{\neg i}) = p(x_i \mid x_{\neg i})$$

We call this method Gibbs Sampling

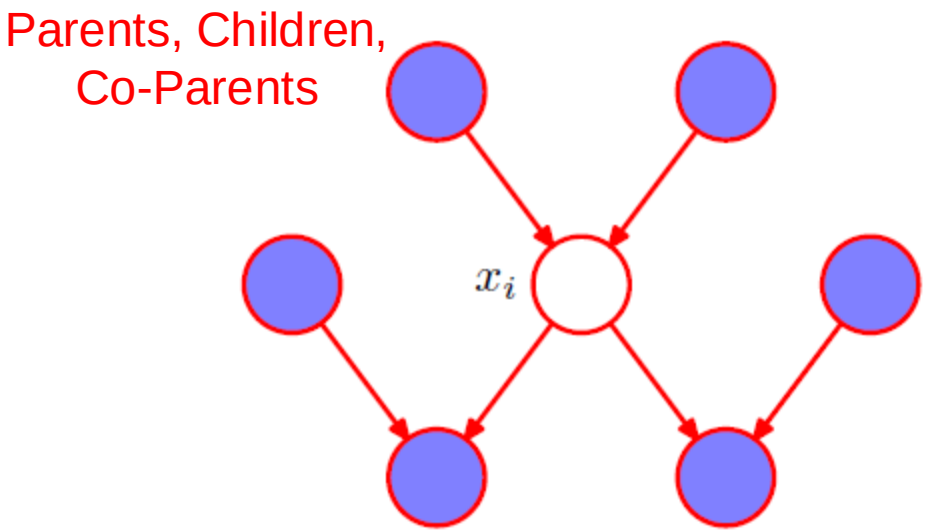
Gibbs Sampling

Recall that an RV is conditionally independent of all RVs given its *Markov Blanket*

MRF



Bayes Net



So complete conditionals only depend on Markov Blanket,

$$p(x_i \mid x_{\neg i}) = p(x_i \mid x_{\mathrm{Mb}(i)})$$

[Source: Bishop, C. PRML]

Consider a set of N variables, z_1, z_1, ...,z_N. Then Gibbs says

Initialize $\left\{ z_i^{(0)} : i = 1,...,N \right\}$

While not_bored

{

For i=1 to N

{

Sample $z_i^{(\tau+1)} \sim p\left(z_i \middle| z_1^{(\tau+1)},...,z_{i-1}^{(\tau+1)},z_{i+1}^{(\tau)},...,z_M^{(\tau)} \right)$

Always accept (i.e., emit $z = z_1^{(\tau+1)},...,z_{i-1}^{(\tau+1)},z_i^{(\tau+1)},z_{i+1}^{(\tau)},...,z_M^{(\tau)}$)

}

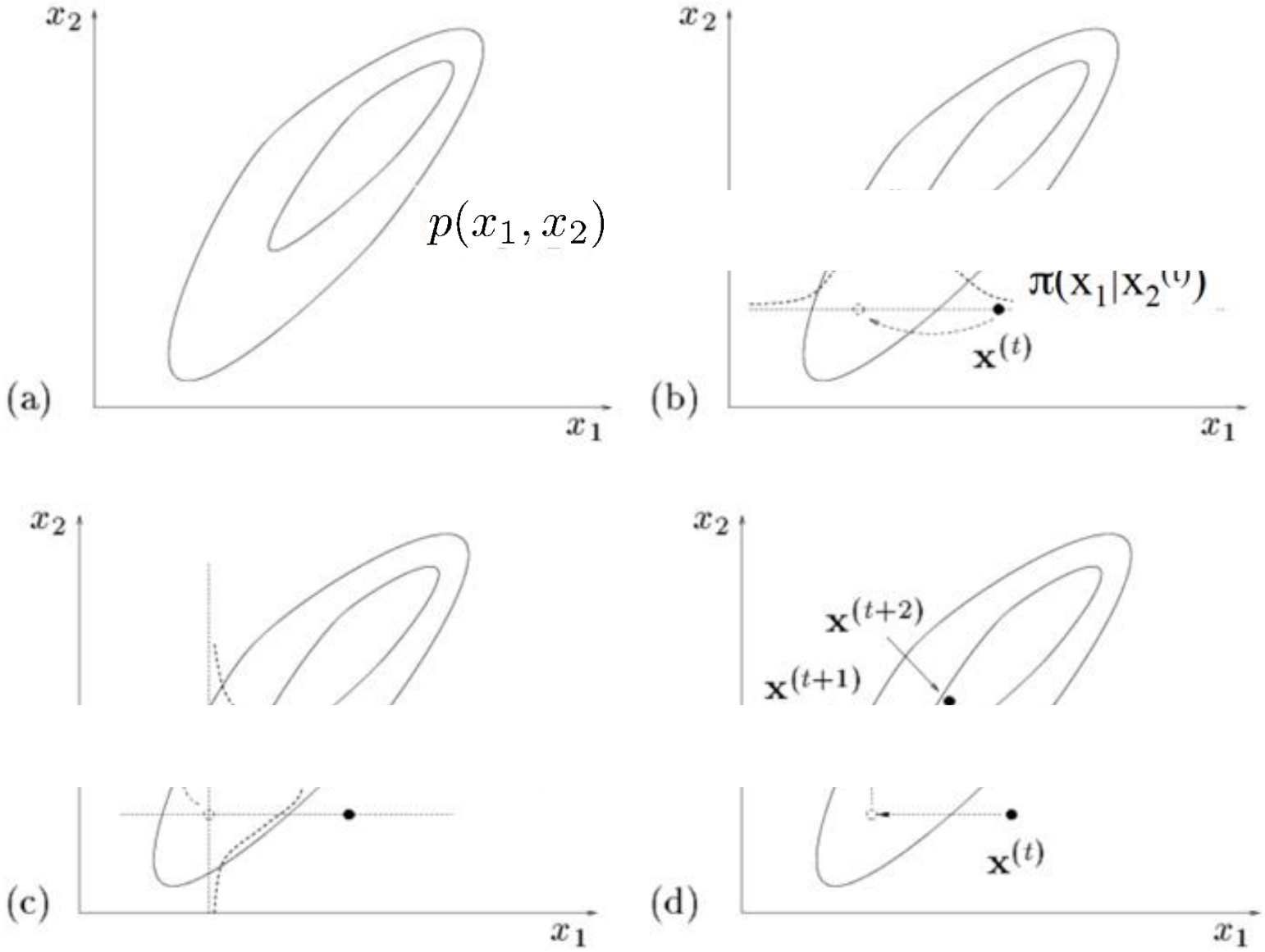
}

Can choose any order (or randomize)

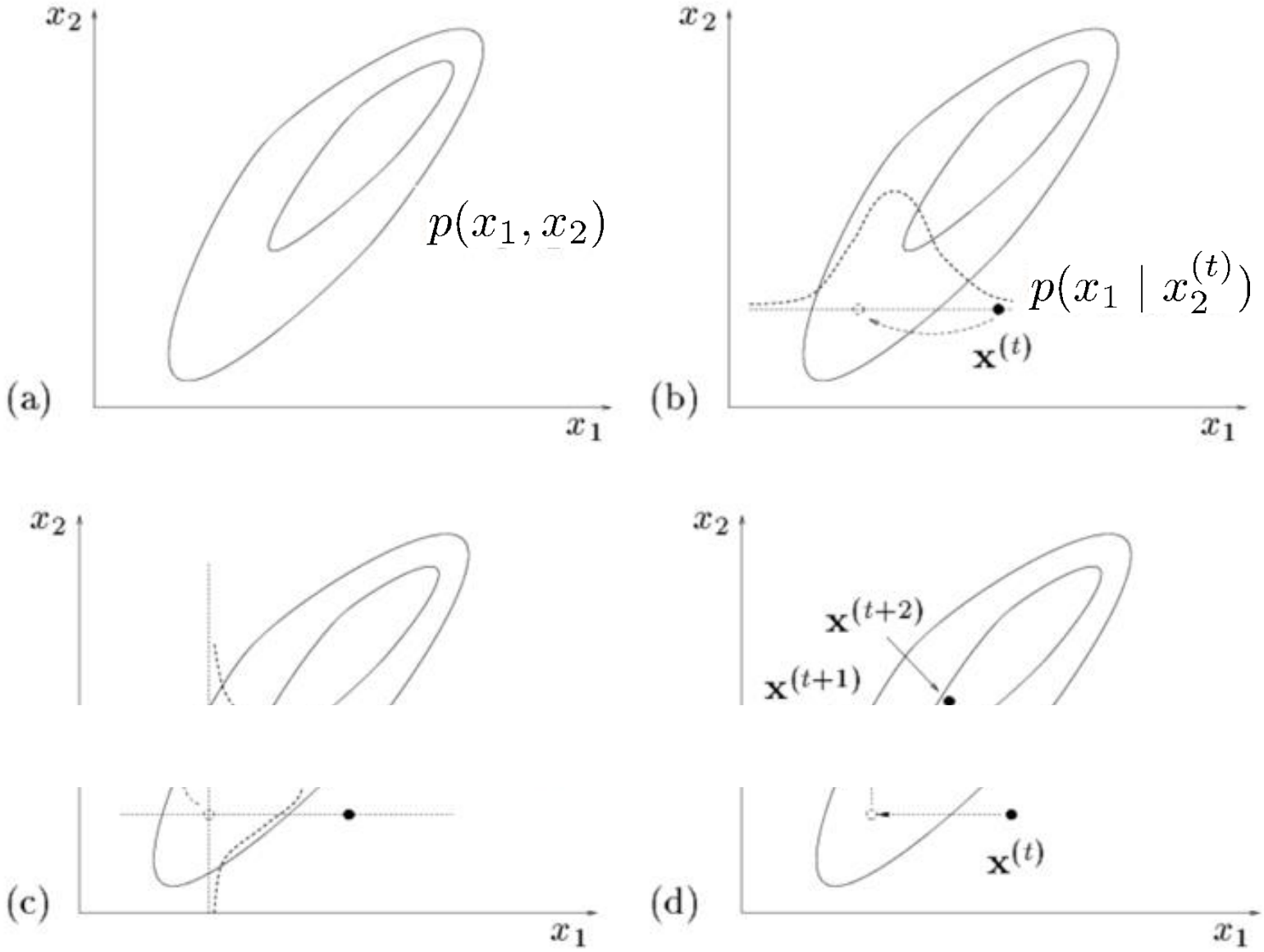
Condition on most recent samples

Gibbs sampling

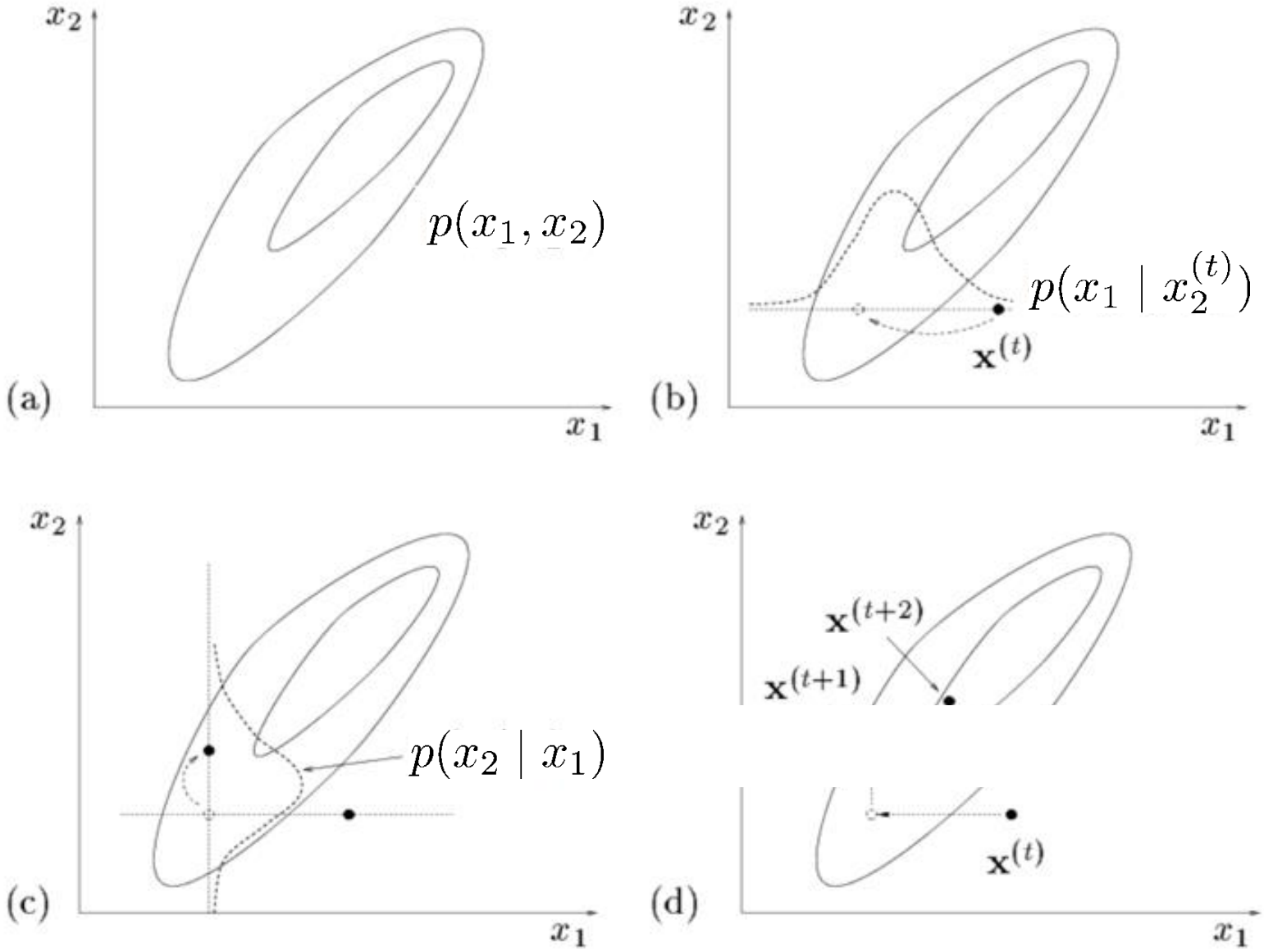
- Gibbs sampling is special case of M-H (but we always accept)
- Unlike M-H we *do not have to choose proposal* $p(z_i \mid z_{\neg i})$
- The proposal distribution will be cycle over
- Transition function T() varies (cycles) over time
  - Relaxation of our assumption used to provide intuition about convergence
  - It still OK because the concatenation of the T() for a cycle converge $p(z_i \mid z_{\neg i})$
- We must be able to compute and sample from
  - This is not always possible in general!
- This is **not** the sample as sampling from the generative model, e.g. Ancestral Sampling in a Bayes Net samples from $p(z_i \mid z_{\mathrm{Pa}(i)})$



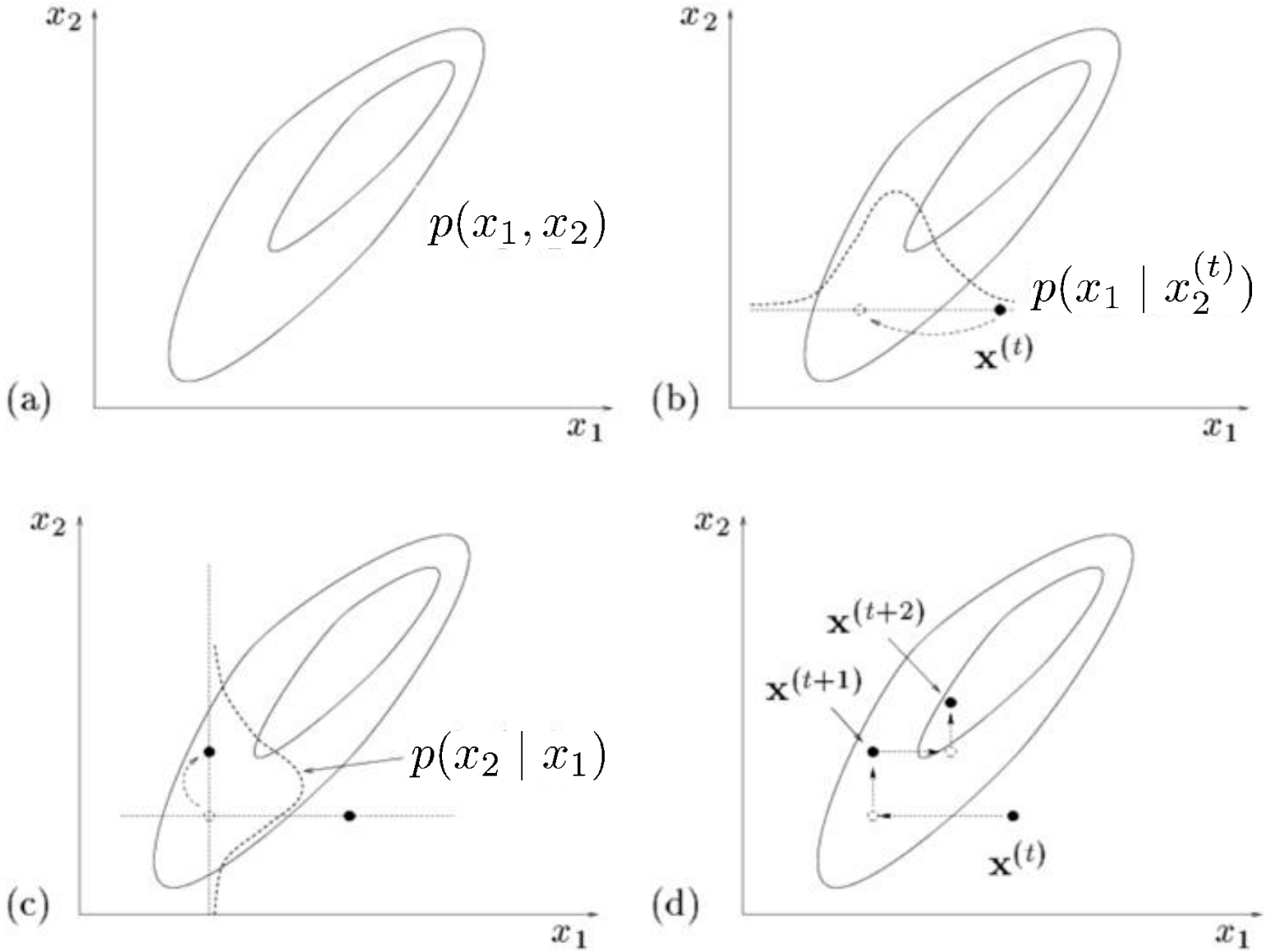
(Source: D. MacKay)



(Source: D. MacKay)



(Source: D. MacKay)



(Source: D. MacKay)

Examples of Gibbs

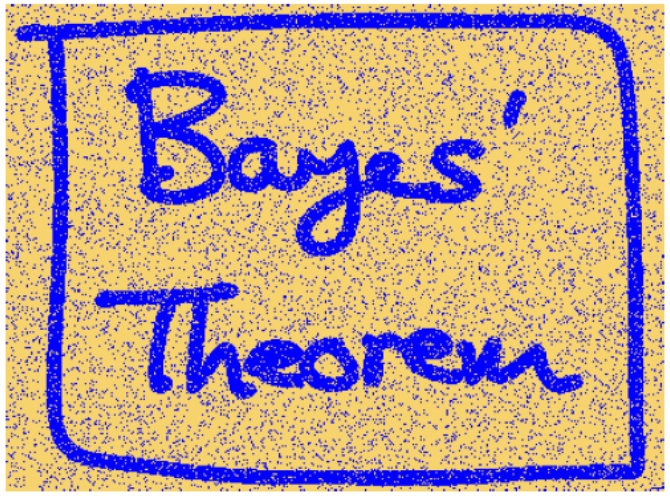
- Gibbs can be very good if one can compute and sample from the complete conditional distributions

- This is often feasible for MRFs of discrete RVs
  - Typical examples include symmetric systems like the Markov random field grids we had for images
  - Complete conditionals only depend on immediate neighboring pixels

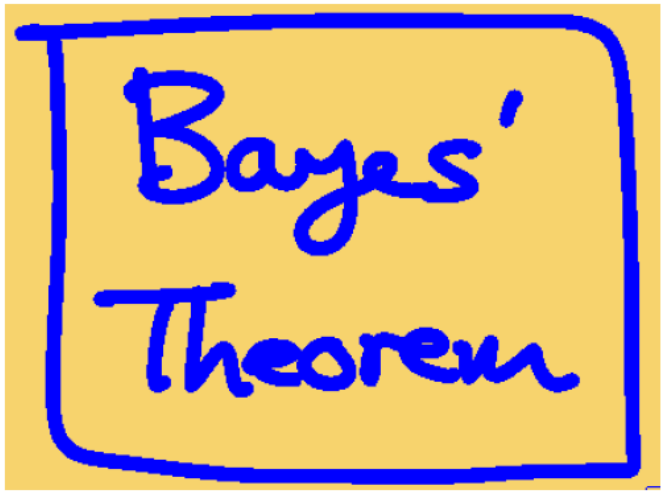
- Continuous models are more complicated, and typically restricted to *exponential family distributions* (we will discuss in the next lecture)

Example: Image Denoising

Noisy Image



Latent Image

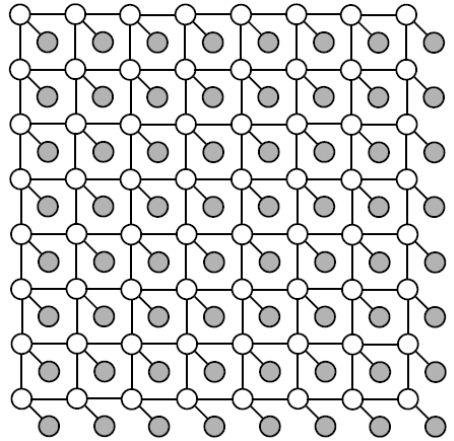


Problem Given observed image corrupted by i.i.d. noise, infer “clean” denoised image.

[Source: Bishop, C. PRML]

Example: Image Denoising

Use a “grid graph” where each pixel is connected to its up/down/left/right neighbors,



$$p(x \mid y) \propto \prod_i \phi_i(x_i, y_i) \prod_{j \in \Gamma(i)} \phi_{ij}(x_i, x_j)$$

Where $x_i, y_i \in \{-1, +1\}$ for convenience

Observation noise

Observation Likelihood: $\log \phi_i(x_i) = \eta x_i y_i$

Pairwise Similarity: $\log \phi_{ij}(x_i, x_j) = \beta x_i x_j$

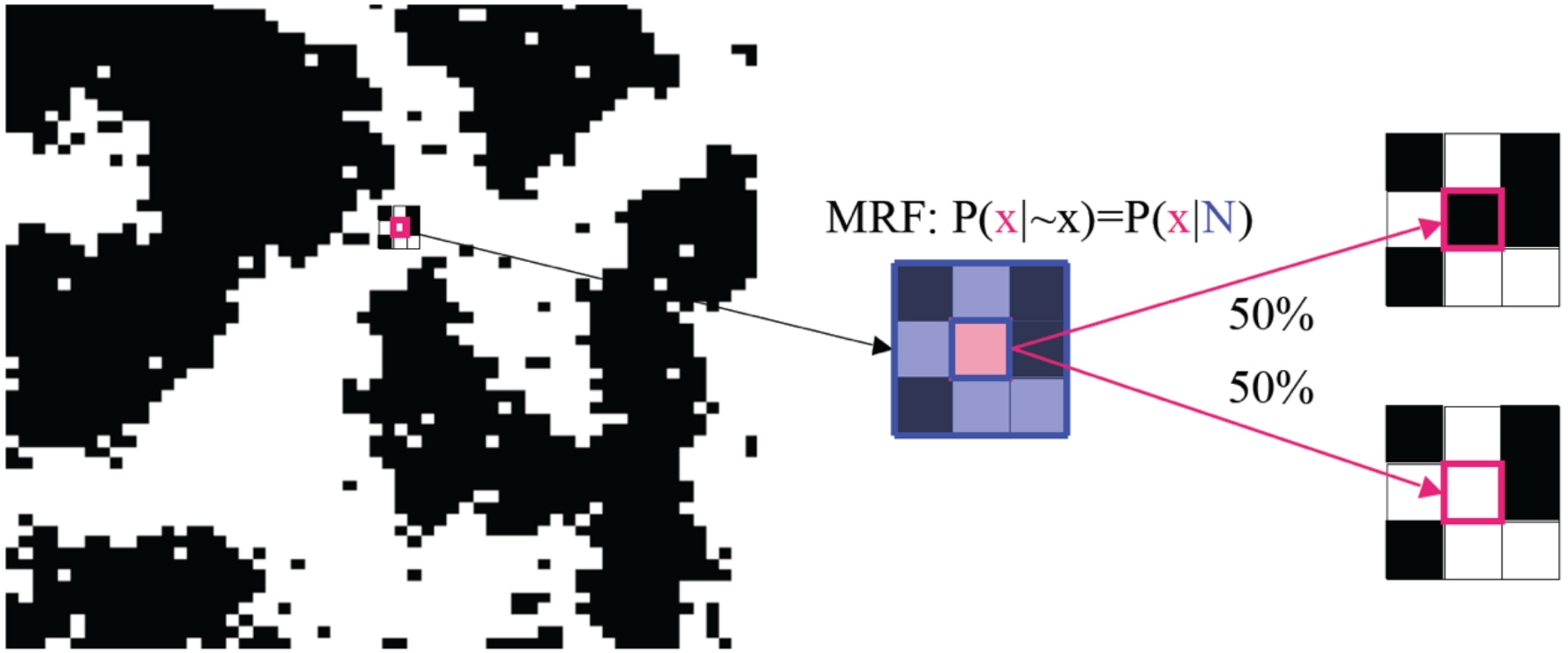
Smoothness prior

Complete conditional only depends on immediate neighbors,

$$p(x_i \mid x_{\neg i}) \propto \phi_i(x_i, y_i) \prod_{j \in \in \Gamma(i)} \phi_{ij}(x_i, x_j)$$

Normalizer only requires summing over 4 neighbors $\mathcal{O}(2^4)$

Examples of Gibbs



(From Dellaert and Zhu tutorial)

Examples of Gibbs

Weak Affinity to Neighbors

Strong Affinity to Neighbors

(From Dellaert and Zhu tutorial)