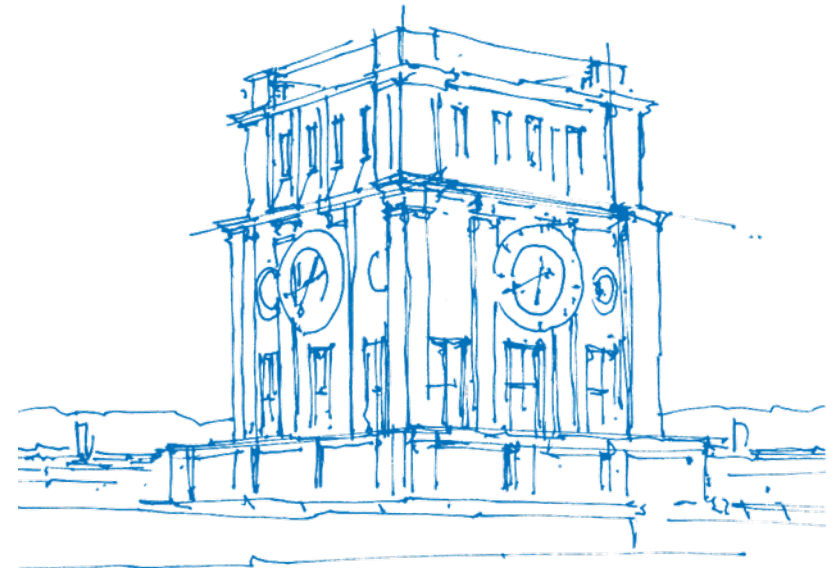




III : Inference on Graphical Models

Tao Wu, Yuesong Shen, Zhenzhang Ye

Computer Vision & Artificial Intelligence
Technical University of Munich

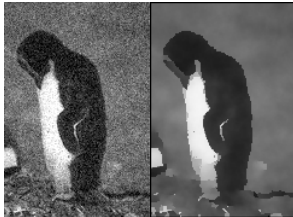


TUM Uhrenturm

Motivation

- Many computer vision tasks boil down to inference on graphical models.

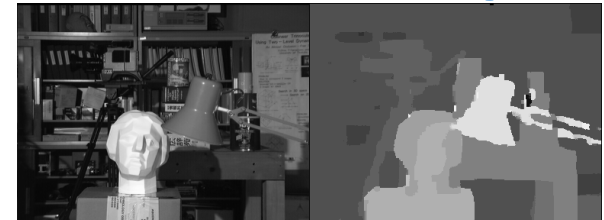
Denoising



Optical flow



Stereo matching



Inpainting



Super-resolution



1. **Probabilistic inference:** compute marginal distribution

$$p(y) = \sum_x p(y, x).$$

2. **MAP inference:** compute maximum of conditional distribution

$$\arg \max_y p(y|x).$$



Exact Inference



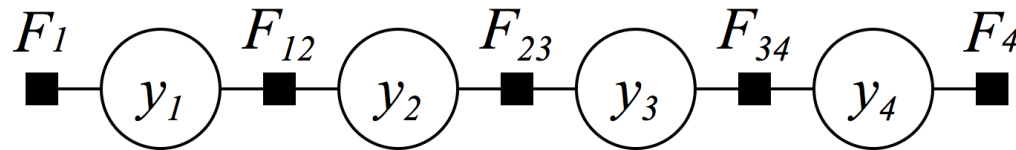
Outline of the Section

- Basic idea: Variable elimination.
- Junction tree algorithm on arbitrary MRFs.
- Belief propagation on tree factor graphs.

Example: Marginal Query on a "Chain" MRF

Joint distribution represented by MRF:

$$p(y_1, y_2, y_3, y_4) = \frac{1}{Z} \phi_1(y_1) \cdot \phi_{12}(y_1, y_2) \cdot \phi_{23}(y_2, y_3) \cdot \phi_{34}(y_3, y_4) \cdot \phi_4(y_4).$$



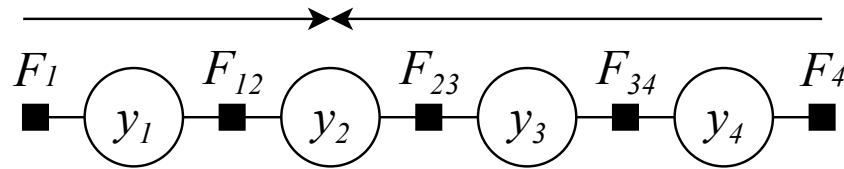
Query about marginal distribution $p(y_2) = ?$

Variable Elimination

Apply **variable elimination** (VE) to the marginal query:

$$\begin{aligned} p(y_2) &= \sum_{y_1, y_3, y_4} p(y_1, y_2, y_3, y_4) \\ &= \sum_{y_1, y_3, y_4} \frac{1}{Z} \phi_1(y_1) \phi_{12}(y_1, y_2) \phi_{23}(y_2, y_3) \phi_{34}(y_3, y_4) \phi_4(y_4) \\ &= \frac{1}{Z} \underbrace{\sum_{y_1} \left(\phi_1(y_1) \phi_{12}(y_1, y_2) \right)}_{=: m_{1 \rightarrow 2}(y_2)} \sum_{y_3} \left(\phi_{23}(y_2, y_3) \underbrace{\sum_{y_4} \left(\phi_{34}(y_3, y_4) \phi_4(y_4) \right)}_{=: m_{4 \rightarrow 3}(y_3)} \right) \\ &= \frac{1}{Z} m_{1 \rightarrow 2}(y_2) \underbrace{\sum_{y_3} \left(\phi_{23}(y_2, y_3) m_{4 \rightarrow 3}(y_3) \right)}_{=: m_{3 \rightarrow 2}(y_2)} \\ &= \frac{1}{Z} m_{1 \rightarrow 2}(y_2) m_{3 \rightarrow 2}(y_2), \\ Z &= \sum_{y_2} m_{1 \rightarrow 2}(y_2) m_{3 \rightarrow 2}(y_2). \end{aligned}$$

Variable Elimination and Beyond



- This algorithm is called **sum-product** VE.
- Sum-product VE yields *exact* inference (of one node marginal) on any *tree-structured factor graph*.
- Observed nodes (a.k.a. *evidence*) can be introduced as reduced factors.
- A similar algorithm can be derived for MAP inference – simply switch all "sum" to "max". The resulting algorithm is called **max-product** VE.
- We shall consider two different extensions beyond VE:
 1. Inference on arbitrary MRFs? \rightsquigarrow **Junction tree algorithm**.
 2. Compute all node/factor marginals at one shot? \rightsquigarrow **Belief propagation**.

Junction Tree

- For an undirected graph $\mathcal{H} = (\mathcal{V}, \mathcal{E})$, the **junction tree** of \mathcal{H} is a tree \mathcal{T} s.t.
 1. The nodes of \mathcal{T} consist of the *maximal cliques* of \mathcal{H} .
 2. The edge S_{ij} between two nodes C_i, C_j of \mathcal{T} (i.e. two maximal cliques of \mathcal{H}) is given by $S_{ij} = C_i \cap C_j$ (known as the *running intersection property*).
- \mathcal{H} is **triangulated** if every cycle of length ≥ 4 has a *chord*. (A chord is an edge that is not part of the cycle but connects two vertices of the cycle.)
- Theorem [Lauritzen '96]: A graph has a junction tree iff it is triangulated.

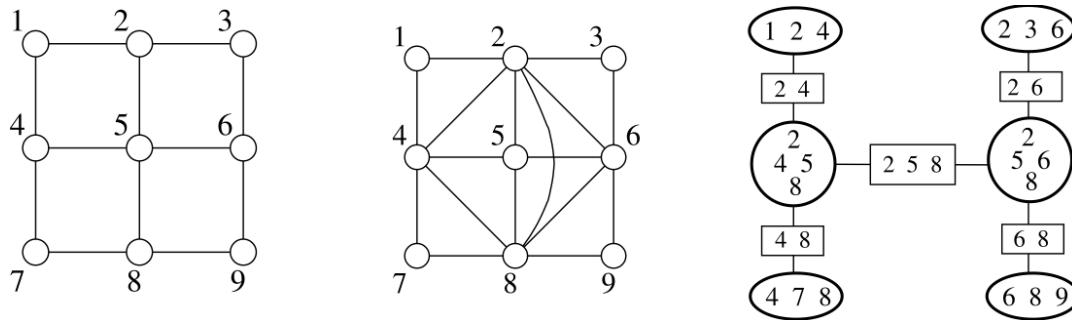
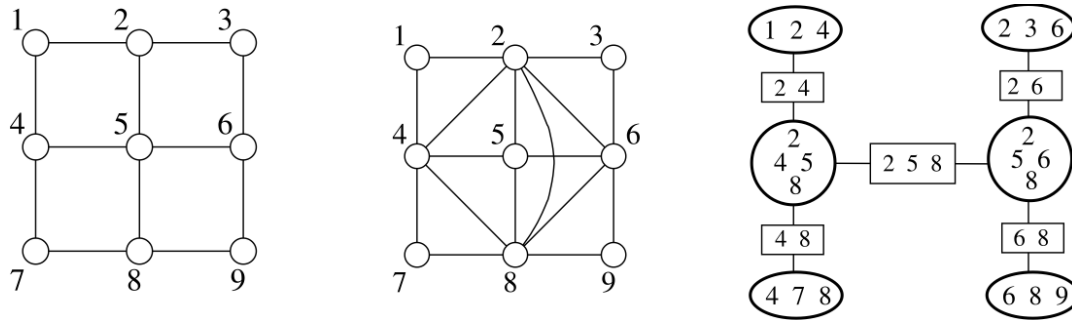


Figure:¹ (a) Original graph; (b) Triangulation of (a); (c) Junction tree for (b).

¹Wainwright and Jordan, “Graphical Models, Exponential Families, and Variational Inference”.
 PGM SS19 : III : Inference on Graphical Models

Junction Tree Algorithm (Sketch)



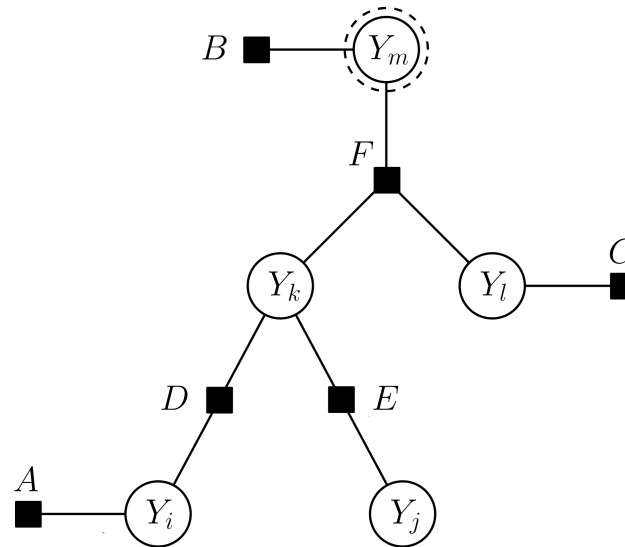
Sum-product message passing on a junction tree \mathcal{T} appears like:

$$m_{C_i \rightarrow C_j}(y_{C_j \cap C_i}) = \sum_{y_{C_i \setminus C_j}} \phi_{C_i}(y_{C_i}) \prod_{C_k \in \text{nbr}_{\mathcal{T}}(C_i) \setminus \{C_j\}} m_{C_k \rightarrow C_i}(y_{C_i \cap C_k}).$$

Overall **junction tree algorithm** for exact inference on an arbitrary MRF:

1. Given a MRF with cycles, triangulate it by adding edges as necessary.
2. Form a junction tree \mathcal{T} for the triangulated MRF.
3. Run VE on the junction tree \mathcal{T} .

Belief Propagation on Tree Factor Graphs²



- Factor graph $\mathcal{G} = (\mathcal{V}, \mathcal{F}, \mathcal{E})$: assumed to be a tree.
- Neighbors of a variable or factor node:

$$\text{nbr}_{\mathcal{G}}(i) = \{F \in \mathcal{F} : (i, F) \in \mathcal{E}\},$$

$$\text{nbr}_{\mathcal{G}}(F) = \{i \in \mathcal{V} : (i, F) \in \mathcal{E}\}.$$

- (Log-domain) energies: $E_F(y_F) = -\log \phi_F(y_F)$.

²Illustrations for BP are extracted from Nowozin & Lampert, 2011.
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BP: Leaf-to-Root Stage

0. Pick $Y_r \in \mathcal{V}$ as the tree root (e.g. Y_m in the figure).

1a. Schedule the leaf-to-root messages.

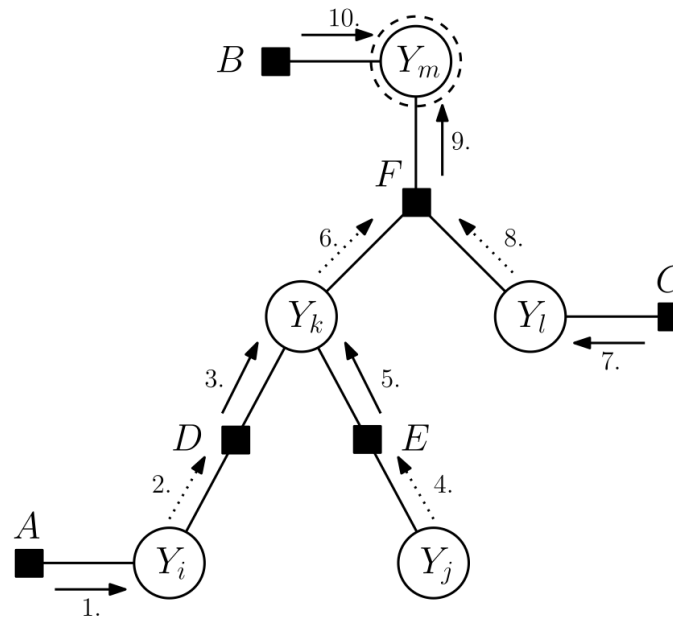


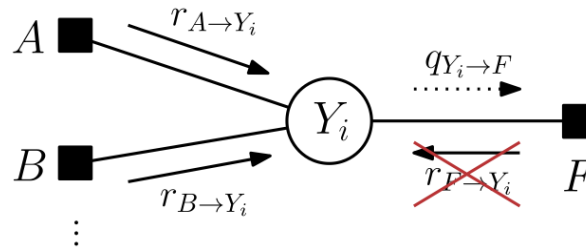
Figure: Belief propagation: leaf-to-root stage.

1b. Compute all leaf-to-root messages (detailed in the next slide).

BP: Compute Messages

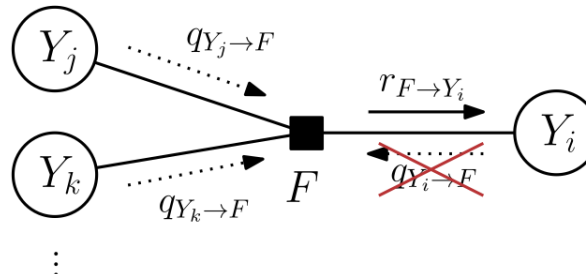
- Compute variable-to-factor message:

$$q_{i \rightarrow F}(y_i) = \sum_{F' \in \text{nbr}_G(i) \setminus \{F\}} r_{F' \rightarrow i}(y_i).$$



- Compute factor-to-variable message:

$$r_{F \rightarrow i}(y_i) = \log \sum_{Y_{F \setminus \{i\}}} \exp \left(-E_F(y_F) + \sum_{i' \in \text{nbr}_G(F) \setminus \{i\}} q_{i' \rightarrow F}(y_{i'}) \right).$$



BP: Compute the Partition Function

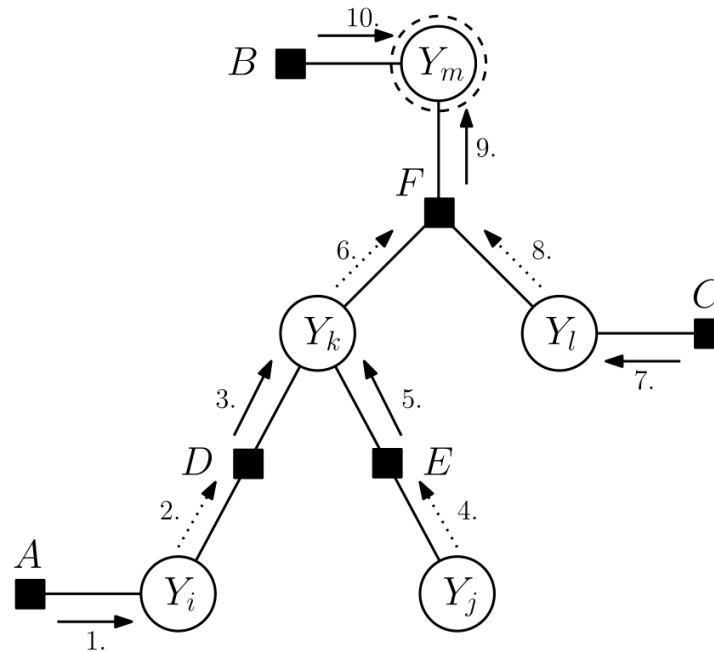


Figure: Belief propagation: leaf-to-root stage.

1c. Compute the log partition function:

$$\log Z = \log \sum_{y_r} \exp \left(\sum_{F \in \text{nbr}_G(r)} r_{F \rightarrow r}(y_r) \right).$$

BP: Root-to-Leaf Stage

2a. Schedule the root-to-leaf messages.

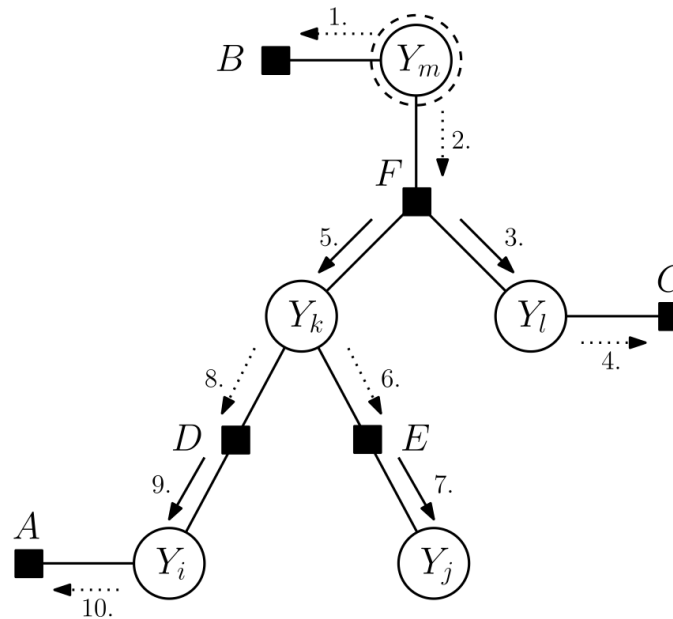


Figure: Belief propagation: root-to-leaf stage.

2b. Compute the root-to-leaf messages using the same formulas on page 12.

BP: Compute Factor / Variable Marginals

2c. Alongside Step 2b, combine messages and compute factor marginals:

$$\mu_F(y_F) := p(y_F) = \exp \left(- E_F(y_F) + \sum_{i \in \text{nbr}_G(F)} q_{i \rightarrow F}(y_i) - \log Z \right),$$

as well as variable marginals:

$$\mu_i(y_i) := p(y_i) = \exp \left(\sum_{F \in \text{nbr}_G(i)} r_{F \rightarrow i}(y_i) - \log Z \right).$$

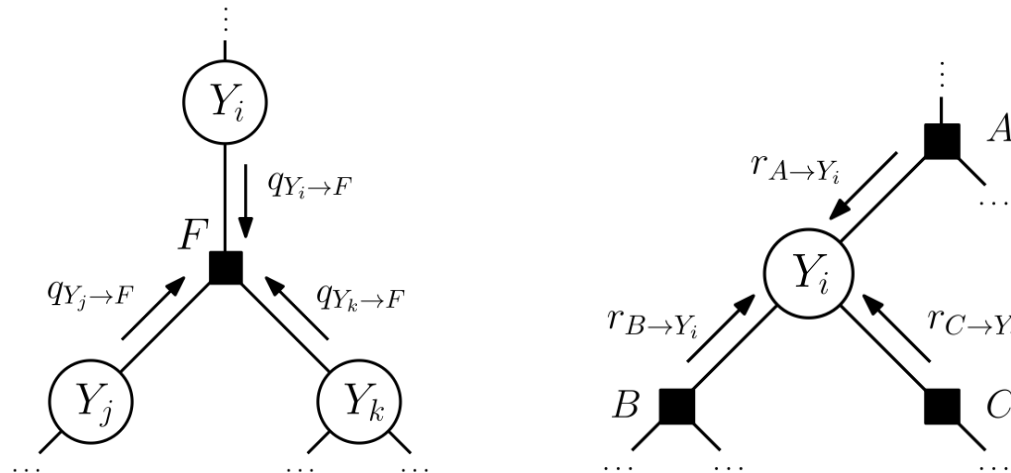


Figure: (left) Factor marginal; (right) Variable marginal.

BP on Pairwise MRFs (as exercise)

For a pairwise MRF $\mathcal{H} = (\mathcal{V}, \mathcal{E})$, the joint distribution is factorized by

$$p(y) = \exp \left(- \sum_{i \in \mathcal{V}} E_i(y_i) - \sum_{(i,j) \in \mathcal{E}} E_{ij}(y_i, y_j) - \log Z \right).$$

BP on such pairwise MRF can be simplified:

- Variable-to-variable message is computed by

$$m_{i \rightarrow j}(y_j) = \log \sum_{y_i} \exp \left(- E_i(y_i) - E_{ij}(y_i, y_j) + \sum_{k \in \text{nbr}_{\mathcal{H}}(i) \setminus \{j\}} m_{k \rightarrow i}(y_i) \right).$$

- Variable marginal is computed by

$$\mu_i(y_i) = \exp \left(- E_i(y_i) + \sum_{k \in \text{nbr}_{\mathcal{H}}(i)} m_{k \rightarrow i}(y_i) - \log Z \right).$$



Further Reading

- Koller & Friedman, Chapters 9, 10.
- Murphy, Chapter 20.
- Nowozin & Lampert, Section 3.1.



Variational Inference



Outline of this Section

- Basic idea: Variational inference.
- Mean field (MF) method.
- Loopy belief propagation (LBP).

Approximation by Tractable Distributions

- Goal: probabilistic inference on joint distribution $p(y)$ represented by *general* MRF (i.e. possibly with loops).
- Instead of tackling the inference on p directly, we first seek for an approximation q within a family \mathcal{Q} consisting of "tractable" distributions:

$$q^* = \arg \min_{q \in \mathcal{Q}} \text{KL}(q | p).$$

- The **Kullback-Leibler (KL) divergence** (a.k.a. *relative entropy*) between two distributions q, p (assuming the "absolute continuity" $q \ll p$) is defined by

$$\text{KL}(q | p) = \sum_y q(y) \log \frac{q(y)}{p(y)}.$$

- Basic properties of KL:
 1. $\text{KL}(q | p) = 0$ iff $p = q$.
 2. $\text{KL}(q | p) \geq 0 \forall q, p$.
 3. $\text{KL}(\cdot | \cdot)$ is not symmetric. Nor does it satisfy the triangle inequality.

Preliminaries to Variational Inference

- Represented by a factor graph $\mathcal{G} = (\mathcal{V}, \mathcal{F}, \mathcal{E})$, p takes the form

$$p(y) = \exp \left(- \sum_{F \in \mathcal{F}} E_F(y_F) - \log Z \right).$$

- Plug p into KL divergence \rightsquigarrow

$$\begin{aligned} \text{KL}(q | p) &= \sum_y q(y) \log \frac{q(y)}{p(y)} = \sum_y q(y) \log q(y) - \sum_y q(y) \log p(y) \\ &= -H(q) + \sum_{F \in \mathcal{F}} \sum_{y_F} \mu_F[q](y_F) E_F(y_F) + \log Z. \end{aligned}$$

- $H(q)$ is the **entropy** of distribution q .
- $\mu_F[q]$ is the marginal distribution of q over variables Y_F .
- $F_{\text{Gibbs}}(q; p) := \text{KL}(q | p) - \log Z = -H(q) + \sum_{F \in \mathcal{F}} \sum_{y_F} \mu_F[q](y_F) E_F(y_F)$ is called the **Gibbs free energy**.
- $\text{KL}(q | p) \geq 0 \Rightarrow \log Z$ is lower bounded by $-F_{\text{Gibbs}}(q; p)$.

Mean Field Approximation

In (naive) **mean field** method, Q consists of q factorized by only unaries:

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

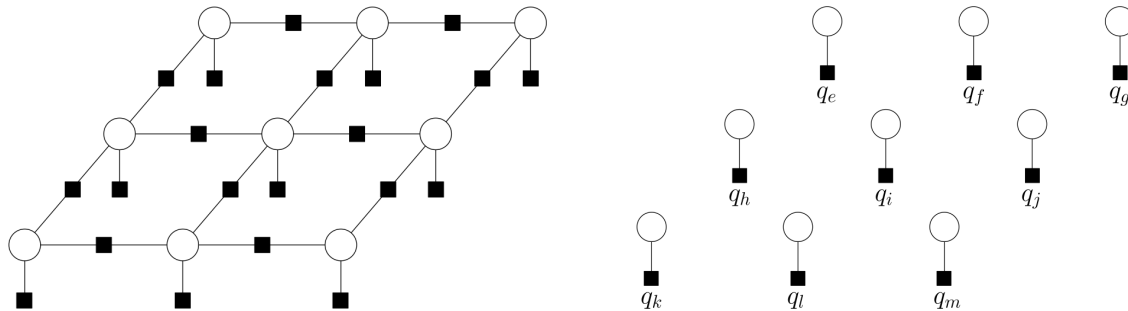


Figure: (left) Original factor graph; (right) (Naive) mean field approximation.

- Such q is "tractable" because $\{q_i(y_i)\}$ provide variable marginals.

- Quick facts:
$$H(q) = \sum_{i \in \mathcal{V}} H(q_i) = - \sum_{i \in \mathcal{V}} \sum_{y_i} q_i(y_i) \log q_i(y_i),$$

$$\mu_F[q](y_F) = \prod_{i \in \text{nbr}_G(F)} q_i(y_i).$$

Mean Field (MF) Approximation

Derivation of MF approximation:

$$\begin{aligned} q^* &= \arg \min_{q \in \mathcal{Q}} \text{KL}(q | p) = \arg \min_{q \in \mathcal{Q}} F(q; p) \\ &= \arg \min_{q \in \mathcal{Q}} -H(q) + \sum_{F \in \mathcal{F}} \sum_{y_F} \mu_F[q](y_F) E_F(y_F) \\ &= \arg \min_{\{q_i\}_{i \in \mathcal{V}}} \sum_{i \in \mathcal{V}} \sum_{y_i} q_i(y_i) \log q_i(y_i) + \sum_{F \in \mathcal{F}} \sum_{y_F} \left(\prod_{i \in \text{nbr}_G(F)} q_i(y_i) \right) E_F(y_F). \end{aligned}$$

Each q_i lies in the probability simplex Δ_i , i.e.

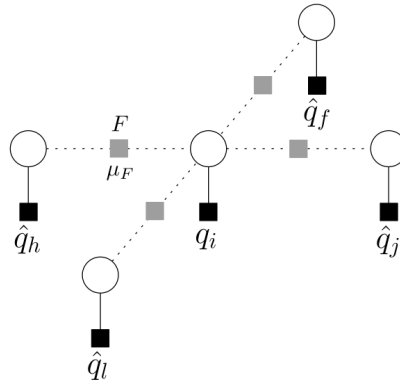
$$\begin{aligned} q_i(y_i) &\geq 0 \quad \forall y_i, \\ \sum_{y_i} q_i(y_i) &= 1. \end{aligned}$$

The optimization can be resolved by *coordinate descent* (next slide).

MF Update Formula

For each block q_i , fix $\hat{q}_{i'}(y_{i'}) = q_{i'}(y_{i'}) \forall i' \neq i$ and solve:

$$q_i^* = \arg \min_{q_i \in \Delta_i} \sum_{y_i} q_i(y_i) \log q_i(y_i) + \sum_{F \in \text{nbr}_{\mathcal{G}}(i)} \sum_{y_F} \left(\prod_{i' \in \text{nbr}_{\mathcal{G}}(F) \setminus \{i\}} \hat{q}_{i'}(y_{i'}) \right) q_i(y_i) E_F(y_F).$$



We obtain an analytical solution via Lagrange multiplier λ for $\sum_{y_i} q_i^*(y_i) = 1$:

$$q_i^*(y_i) = \exp \left(-1 - \sum_{F \in \text{nbr}_{\mathcal{G}}(i)} \sum_{y_{F \setminus \{i\}}} \left(\prod_{i' \in \text{nbr}_{\mathcal{G}}(F) \setminus \{i\}} \hat{q}_{i'}(y_{i'}) \right) E_F(y_F) + \lambda \right)$$

$$\propto \exp \left(- \sum_{F \in \text{nbr}_{\mathcal{G}}(i)} \sum_{y_{F \setminus \{i\}}} \left(\prod_{i' \in \text{nbr}_{\mathcal{G}}(F) \setminus \{i\}} \hat{q}_{i'}(y_{i'}) \right) E_F(y_F) \right).$$

Some Remarks on MF

- The term $\prod_{i' \in \text{nbr}_{\mathcal{G}}(F) \setminus \{i\}} \hat{q}_{i'}(y_{i'})$ is taken to be 1 if $\text{nbr}_{\mathcal{G}}(F) \setminus \{i\} = \emptyset$.
- For a pairwise MRF \mathcal{H} , the MF update rule can be simplified as

$$q_i^*(y_i) \propto \exp \left(- E_i(y_i) - \sum_{j \in \text{nbr}_{\mathcal{H}}(i)} \sum_{y_j} \hat{q}_j(y_j) E_{ij}(y_i, y_j) \right).$$

- MF is an iterative procedure which converges to a *locally optimal* solution q^* .
- Upon convergence, $\{q_i^*\}$ directly provide (approximate) variable marginals.
- The tractable family \mathcal{Q} can be more sophisticated than factorizations of unaries in naive mean field. \rightsquigarrow *Structured mean field* approximation.



From Belief Propagation to Loopy Belief Propagation

- Previously we have seen how belief propagation works on tree factor graphs.
- We can use similar update rules to derive **loopy belief propagation** (LBP).
- Although LBP does not guarantee the convergence (if at all) to the true marginal, it often performs well and is widely used in practice³.
- In the following, we first present the LBP algorithm and then interpret it from perspective of variational inference.

³Murphy et al., “Loopy Belief Propagation for Approximate Inference: An Empirical Study”.
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Loopy Belief Propagation

On a factor graph $\mathcal{G} = (\mathcal{V}, \mathcal{F}, \mathcal{E})$, LBP proceeds as follows.

0. Initialize all variable-to-factor messages: $q_{i \rightarrow F}(y_i) = 0$. Then iterate:

1. Compute all factor-to-variable messages:

$$r_{F \rightarrow i}(y_i) = \log \sum_{y_{F \setminus \{i\}}} \exp \left(- E_F(y_F) + \sum_{i' \in \text{nbr}_{\mathcal{G}}(F) \setminus \{i\}} q_{i' \rightarrow F}(y_{i'}) \right).$$

2. Compute all (normalized) variable-to-factor messages:

$$\begin{aligned} \bar{q}_{i \rightarrow F}(y_i) &= \sum_{F' \in \text{nbr}_{\mathcal{G}}(i) \setminus \{F\}} r_{F' \rightarrow i}(y_i), \\ \delta_{i \rightarrow F} &= \log \sum_{y_i} \exp \left(\bar{q}_{i \rightarrow F}(y_i) \right), \\ q_{i \rightarrow F}(y_i) &= \bar{q}_{i \rightarrow F}(y_i) - \delta_{i \rightarrow F}. \end{aligned}$$

Loopy Belief Propagation (cont'd)

3. Compute all factor marginals:

$$\mu_F(y_F) \propto \exp \left(- E_F(y_F) + \sum_{i \in \text{nbr}_G(F)} q_{i \rightarrow F}(y_i) \right).$$

4. Compute all variable marginals:

$$\mu_i(y_i) \propto \exp \left(\sum_{F \in \text{nbr}_G(i)} r_{F \rightarrow i}(y_i) \right).$$

Differences compared to BP:

- The normalization constants in the computation of marginals differ at each factor/variable.
- The log partition function is not directly available, but it can be approximated by the **Bethe free energy**:

$$\begin{aligned} -\log Z \approx F_{\text{Bethe}}(\mu; \rho) := & \sum_{i \in \mathcal{V}} (1 - |\text{nbr}_G(i)|) \sum_{y_i} \mu_i(y_i) \log \mu_i(y_i) \\ & + \sum_{F \in \mathcal{F}} \sum_{y_F} \mu_F(y_F) \left(E_F(y_F) + \log \mu_F(y_F) \right). \end{aligned}$$

Interpretation of LBP

On a pairwise MRF $\mathcal{H} = (\mathcal{V}, \mathcal{E})$, LBP can be interpreted as an attempt to solve:

$$\begin{aligned} \text{minimize}_{\{\mu_i\}_{i \in \mathcal{V}}, \{\mu_{ij}\}_{(i,j) \in \mathcal{E}}} & \sum_{i \in \mathcal{V}} (1 - |\text{nbr}_{\mathcal{H}}(i)|) \sum_{y_i} \mu_i(y_i) \log \mu_i(y_i) \\ & + \sum_{(i,j) \in \mathcal{E}} \sum_{y_i, y_j} \mu_{ij}(y_i, y_j) \left(E_{ij}(y_i, y_j) + \log \mu_{ij}(y_i, y_j) \right) \end{aligned}$$

$$\text{subject to } \mu_i(y_i) \geq 0, \mu_{ij}(y_i, y_j) \geq 0, \sum_{y_i} \mu_i(y_i) = 1, \sum_{y_i} \mu_{ij}(y_i, y_j) = \mu_j(y_j).$$

- The constraints impose *local consistency* between node marginals $\{\mu_i\}$ and edge marginals $\{\mu_{ij}\}$.
- However, $\{\mu_i\}, \{\mu_{ij}\}$ under these constraints are may not be marginals of any joint distribution on \mathcal{H} (i.e. outer approximation of *marginal polytope*).
- An iterative algorithm for the constrained optimization can recover LBP updates.
- An amazing theory on variational inference arise in this context — we point those interested to the "monster" paper [Jordan & Wainwright, 2008].

LBP vs. MF

- (+) (Naive) MF optimizes over only variable marginals; LBP optimizes over variable and factor marginals under local consistency constraints.
- (+) LBP does exact inference on factor graphs without loops; MF is exact on a strict subclass of factor graphs, on which all true factor marginals are factorized by $\mu_F(y_F) = \prod_{i \in \text{nbr}_G(F)} \mu_i(y_i)$ (hence an inner approximation of marginal polytope).
- (+) While both being approximate inference techniques, LBP tends to be more accurate than MF in practice.
- (−) MF provides a lower bound of the log partition function (given by negative Gibbs free energy), while LBP does not.
- (−) Compared to LBP, it is easier to extend MF to distributions other than discrete and Gaussian, due to the simplicity of working with only variable marginals.



Further Reading

- Murphy, Chapters 21, 22.
- Nowozin & Lampert, Sections 3.2, 3.3.
- Koller & Friedman, Chapter 11.
- Jordan & Wainwright, Chapters 4, 5.



Sampling-based Inference



Outline of the Section

- Monte Carlo (MC) method.
- Markov chain Monte Carlo (MCMC) method.
- Sampling of Bayesian network and Markov random field.

Basic Principle of Sampling

Given a distribution p , we can approximate p using a finite sequence of **samples** $\{x_n\}_{n=1}^N$ in the sense that:

$$\mathbb{E}_{x \sim p}[f(x)] = \sum_x f(x)p(x) \approx \frac{1}{N} \sum_{n=1}^N f(x_n) \quad \text{for any function } f.$$

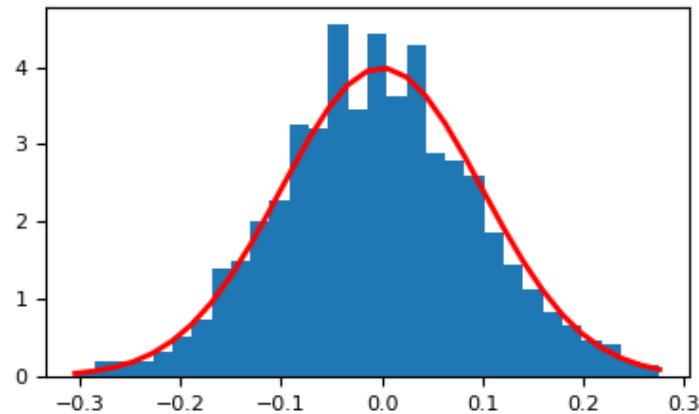


Figure: Sampling of a Gaussian⁴.

⁴<https://docs.scipy.org/doc/numpy/reference/generated/numpy.random.normal.html>

Pseudo-Random Number Generator

Linear congruential generator for sampling $\text{Unif}(0, 1)$:

$$x_{n+1} = (a \cdot x_n + c) \pmod{m}.$$

- Most fundamental sampler above all.
- The generated samples are *pseudo-random* — $\{x_n\}$ are "deterministic" if the generator (i.e. parameters a, c, m) and the *seed* x_0 are fixed.

Source	modulus m	multiplier a	increment c	output bits of seed in <i>rand()</i> or <i>Random(L)</i>
<i>Numerical Recipes</i>	2^{32}	1664525	1013904223	
Borland C/C++	2^{32}	22695477	1	bits 30..16 in <i>rand()</i> , 30..0 in <i>irand()</i>
glibc (used by GCC) ^[9]	2^{31}	1103515245	12345	bits 30..0
ANSI C: Watcom, Digital Mars, CodeWarrior, IBM VisualAge C/C++ ^[10] C90, C99, C11: Suggestion in the ISO/IEC 9899 ^[11] , C18	2^{31}	1103515245	12345	bits 30..16
Borland Delphi, Virtual Pascal	2^{32}	134775813	1	bits 63..32 of (<i>seed</i> * <i>L</i>)
Turbo Pascal	2^{32}	134775813 (0x8088405 ₁₆)	1	
Microsoft Visual/Quick C/C++	2^{32}	214013 (343FD ₁₆)	2531011 (269EC3 ₁₆)	bits 30..16
Microsoft Visual Basic (6 and earlier) ^[12]	2^{24}	1140671485 (43FD43FD ₁₆)	12820163 (C39EC3 ₁₆)	
RtlUniform from Native API ^[13]	$2^{31} - 1$	2147483629 (7FFFFFFD ₁₆)	2147483587 (7FFFFFFC3 ₁₆)	
Apple CarbonLib, C++11's <i>minstd_rand0</i> ^[14]	$2^{31} - 1$	16807	0	see <i>MINSTD</i>
C++11's <i>minstd_rand</i> ^[14]	$2^{31} - 1$	48271	0	see <i>MINSTD</i>
MMIX by Donald Knuth	2^{64}	6364136223846793005	1442695040888963407	
Newlib, Musl	2^{64}	6364136223846793005	1	bits 63..32
VMS's <i>MTHSRANDOM</i> , ^[15] old versions of glibc	2^{32}	69069 (10DCD ₁₆)	1	
Java's <i>java.util.Random</i> , POSIX <i>[ln]rand48</i> , glibc <i>[ln]rand48_r</i>	2^{48}	25214903917 (5DEECE66D ₁₆)	11	bits 47...16

Figure: Common used linear congruential generators⁵.

⁵https://en.wikipedia.org/wiki/Linear_congruential_generator

Sampling Gaussians

- Sample univariate Gaussian distribution by **Box-Muller method**:
 1. Sample $(z_1, z_2) \sim p_z(z_1, z_2) = \frac{1}{\pi} \mathbf{1}\{z_1^2 + z_2^2 \leq 1\}$ (i.e. uniform distribution supported on the unit 2D circle).
 2. Perform the Box-Muller transformation and output x_1, x_2 :

$$x_i = z_i \sqrt{\frac{-2 \log(z_1^2 + z_2^2)}{z_1^2 + z_2^2}}, \quad i \in \{1, 2\}.$$

Fact: x_1, x_2 are two independent samples of $\text{Normal}(0, 1)$:

$$p_x(x_1, x_2) = p_z(z_1, z_2) \left| \frac{\partial(z_1, z_2)}{\partial(x_1, x_2)} \right| = \frac{1}{\sqrt{2\pi}} \exp(-x_1^2/2) \cdot \frac{1}{\sqrt{2\pi}} \exp(-x_2^2/2).$$

- Sample multivariate Gaussian distribution, $y \sim \text{Normal}(\mu, \Sigma)$, by:
 1. Perform Cholesky decomposition $\Sigma = LL^\top$.
 2. Sample $x \sim \text{Normal}(0, I)$, and output $y := Lx + \mu$.

Fact: $\mathbb{E}[y] = \mu$, and $\text{Var}[y] = L \text{Var}[x] L^\top = LIL^\top = \Sigma$.

Sampling by Inverse CDF

Sample a distribution via **inverse Cumulative Distribution Function**:

- Let $U \sim \text{Unif}(0, 1)$ and F_p be the CDF for (univariate) distribution p , i.e.

$$F_p(y) := \int_{-\infty}^y p(x) dx = \int_{-\infty}^{\infty} \mathbf{1}\{x \leq y\} p(x) dx.$$

- Note that $X \sim p \Leftrightarrow P(X \leq y) = F_p(y)$.

- We assert $F_p^{-1}(U) \sim p$, since

$$\begin{aligned} P(F_p^{-1}(U) \leq y) &= P(U \leq F_p(y)) && \text{(since } F_p \text{ is monotone)} \\ &= F_p(y). && \text{(since } P(U \leq u) = u \ \forall u \in [0, 1]) \end{aligned}$$

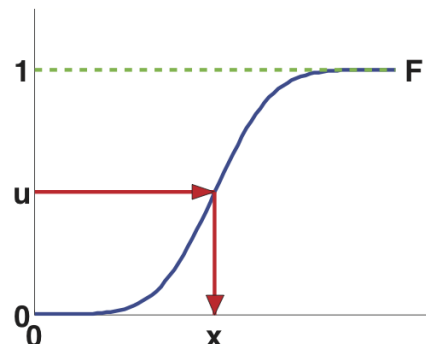


Figure: Sampling using inverse CDF [Murphy, Figure 23.1].

Rejection Sampling

- Inverse CDF sampling requires explicit knowledge of F_p^{-1} .
- **Rejection Sampling:**
Require: *unnormalized* target distribution \tilde{p} (i.e. $\tilde{p}(x)/Z_p = p(x)$ for target distribution p), *proposal distribution* q and constant $M > 0$ s.t. $Mq(x) \geq \tilde{p}(x) \forall x (\Rightarrow p \ll q)$.
1. Sample $x \sim q$, and $u \sim \text{Unif}(0, 1)$.
2. If $u > \frac{\tilde{p}(x)}{Mq(x)}$, reject the proposed sample x ; otherwise, accept x .

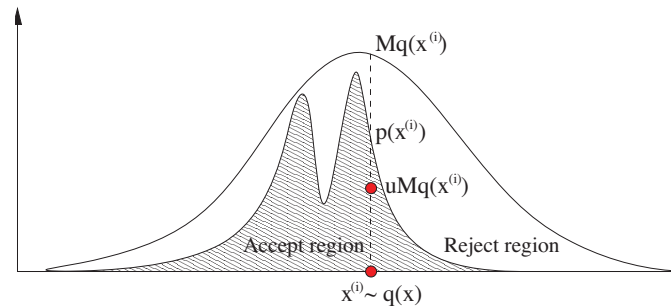


Figure: Rejection sampling [Murphy, Figure 23.2].

- Proof: (univariate case) $P(x \leq y | x \text{ accepted}) = \frac{P(x \leq y, x \text{ accepted})}{P(x \text{ accepted})} = \frac{\int \int \mathbf{1}\{u \leq \tilde{p}(x)/(Mq(x)), x \leq y\} q(x) du dx}{\int \int \mathbf{1}\{u \leq \tilde{p}(x)/(Mq(x))\} q(x) du dx} = \frac{\frac{1}{M} \int_{-\infty}^y \tilde{p}(x) dx}{\frac{1}{M} \int_{-\infty}^{\infty} \tilde{p}(x) dx} = F_p(y)$.

Importance Sampling

- In rejection sampling, $P(x \text{ accepted}) = \frac{1}{M} \int_{-\infty}^{\infty} \tilde{p}(x) dx$, i.e., many proposed samples are potentially wasted.
- In contrast, **importance sampling** uses all samples by weighting them:

$$\mathbb{E}_{x \sim p}[f(x)] = \int f(x) \frac{p(x)}{q(x)} q(x) dx \approx \frac{1}{N} \sum_{n=1}^N w_n f(x_n),$$

with $x_n \sim q$ i.i.d. and $w_n = \frac{p(x_n)}{q(x_n)}$.

- Extend importance sampling to *unnormalized* distributions \tilde{p} , \tilde{q} :

$$\mathbb{E}_{x \sim p}[f(x)] = \frac{Z_q}{Z_p} \int f(x) \frac{\tilde{p}(x)}{\tilde{q}(x)} q(x) dx \approx \frac{Z_q}{Z_p} \frac{1}{N} \sum_{n=1}^N \frac{\tilde{p}(x_n)}{\tilde{q}(x_n)} f(x_n), \quad x_n \sim q \text{ i.i.d.}$$

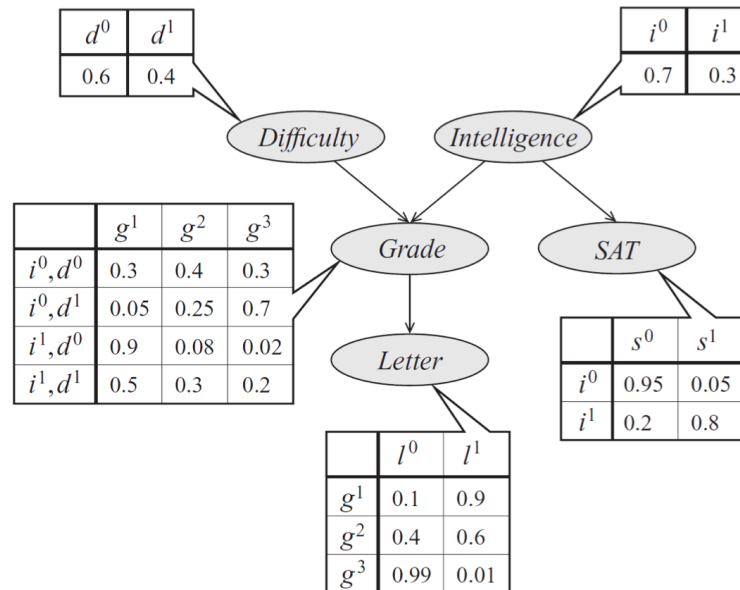
$$\frac{Z_p}{Z_q} = \int \frac{1}{Z_q} \tilde{p}(x) dx = \int \frac{\tilde{p}(x)}{\tilde{q}(x)} q(x) dx \approx \frac{1}{N} \sum_{n=1}^N \frac{\tilde{p}(x'_n)}{\tilde{q}(x'_n)}, \quad x'_n \sim q \text{ i.i.d.}$$

We often take $x'_n = x_n$. For finite N , this yields a *biased estimator* of p .

Sampling of Bayesian Network

Recall that the distribution represented by BN is given by

$$p(x) = \prod_{i \in \mathcal{V}} p(x_i | (x_j)_{j \in \text{Pa}_G(i)}).$$



Ancestral sampling: Given that no variables are observed, we can follow the topological order of the BN and sample each individual conditional distribution.

Sampling of BN with Evidence

In case the BN \mathcal{G} contains observed nodes (called **evidence**), we can modify ancestral sampling (AS) as follows:

- **Logic sampling**: Perform AS. Whenever a sampled node takes different value from the evidence, reject the whole sample and start again.
- LS is closely related to rejection sampling. Unsurprisingly, it is inefficient for wasting samples.
- **Likelihood weighting**: Perform AS. Whenever node i is observed (written $i \in \mathcal{O}$), we *clamp* the observed value \bar{x}_i and *weight* the whole sample by the probability of the clamped node $p(\bar{x}_i | x_{\text{Pa}_{\mathcal{G}}(i)})$.
- LW can be interpreted as importance sampling with weights given by:

$$w(x) = \frac{p(x)}{q(x)} = \frac{\prod_{i \in \mathcal{V}} p(x_i | x_{\text{Pa}_{\mathcal{G}}(i)})}{\prod_{i \in \mathcal{V} \setminus \mathcal{O}} p(x_i | x_{\text{Pa}_{\mathcal{G}}(i)}) \prod_{i \in \mathcal{O}} \delta_{\bar{x}_i}(x_i)} = \prod_{i \in \mathcal{O}} p(\bar{x}_i | x_{\text{Pa}_{\mathcal{G}}(i)}).$$

$\delta_{\bar{x}}$ denotes the **Dirac distribution** defined by $\delta_{\bar{x}}(x) = \begin{cases} 1 & \text{if } x = \bar{x}, \\ 0 & \text{otherwise.} \end{cases}$

Towards Markov Chain Monte Carlo

- Monte Carlo sampling requires exact or rough knowledge of the partition function (of a MRF), hence impractical for high dimensional distributions.
- Instead of generating i.i.d. samples, **Monte Carlo Markov Chain** (MCMC) constructs a *Markov chain* using "*adaptive*" *proposal distributions*, in a way that the Markov chain converges to a *stationary distribution* identical to the target distribution.

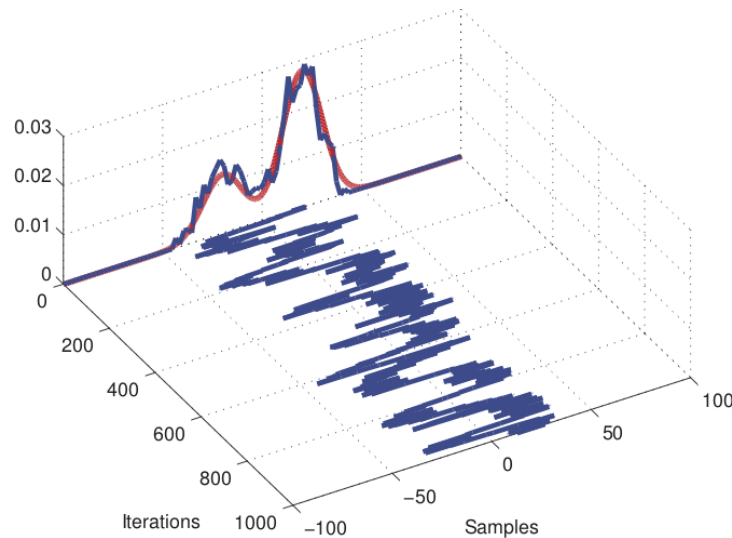


Figure: Sampling by MCMC [Murphy, Figure 24.7].

Markov Chain

- The (discrete-time) **Markov chain** (MC) is a sequence of RVs $(X_n)_{n=1}^{\infty}$ satisfying the Markov property:

$$P(X_{n+1} = x | X_1, \dots, X_n \text{ given}) = P(X_{n+1} = x | X_n \text{ given}).$$

"The future depends on the past only through the present."

- Further assume:
 1. All X_n has a *finite state space* \mathcal{X} .
 2. The MC is *time-homogeneous*, i.e., the transition probability is time-independent

$$P(X_{n+1} = x' | X_n = x) =: \pi(x' | x) \quad \forall n,$$

with $\pi(x' | x) \geq 0$, $\sum_{x'} \pi(x' | x) = 1$. π is the **transition kernel** of the MC.

- Denote by p_n the distribution at time step n :

$$p_n(x) = P(X_n = x) \quad \Rightarrow \quad p_{n+1}(x') = \sum_x p_n(x) \pi(x' | x).$$

Relevant Notions on Markov Chain

- p_* is a **stationary distribution** for the MC if

$$p_*(x') = \sum_x p_*(x)\pi(x'|x) \quad \forall x' \in \mathcal{X}.$$

- The MC is **irreducible** if

$$\forall x, x' \in \mathcal{X} \quad \exists n(x, x') \text{ s.t. } P(X_n = x' | X_0 = x) > 0,$$

i.e., it is possible to get to any state from any state in finite steps.

- A state $x \in \mathcal{X}$ has *period* T_x if

$$T_x = \gcd\{n > 0 : P(X_n = x | X_0 = x) > 0\},$$

i.e., any loop over state x must occur in a multiple of T_x steps.

We say the MC is **aperiodic** if $T_x = 1 \quad \forall x \in \mathcal{X}$.

- The MC is **regular** if

$$\exists n \text{ s.t. } P(X_n = x' | X_0 = x) > 0 \quad \forall x, x' \in \mathcal{X}.$$

Fact: MC is regular \Rightarrow MC is irreducible and aperiodic.

Convergence to Stationary Distribution

Theorem 1: If the transition kernel π of a Markov chain satisfies the *detailed balance condition* for some distribution p_* :

$$p_*(x)\pi(x'|x) = p_*(x')\pi(x|x') \quad \forall x, x' \in \mathcal{X},$$

then p_* is a stationary distribution for the Markov chain.

Proof: $\sum_x p_*(x)\pi(x'|x) = \sum_x p_*(x')\pi(x|x') = p_*(x') \sum_x \pi(x|x') = p_*(x')$.

Theorem 2⁶: Every irreducible, aperiodic, finite-state Markov chain has a limiting distribution

$$p_*(x') = \lim_{n \rightarrow \infty} \sum_x P(X_n = x' | X_0 = x) p_0(x),$$

regardless of the initial distribution p_0 . Indeed, p_* is equal to the unique stationary distribution of the MC.

⁶[Murphy, Theorem 17.2.1]

Metropolis-Hastings Algorithm

Metropolis-Hastings (MH) algorithm:

Input: unnormalized target distribution \tilde{p} (i.e. $p_*(x) = \tilde{p}(x)/Z_p$), proposal distribution $q(\cdot|\cdot)$, initial sample x_0 . Loop $n = 0, 1, 2, \dots$ as follows:

1. Set $x = x_n$. Sample $x' \sim q(x'|x)$.
2. Compute acceptance probability $\alpha = \frac{\tilde{p}(x')q(x|x')}{\tilde{p}(x)q(x'|x)}$.
3. Compute $r = \min(1, \alpha)$. Sample $u \sim \text{Unif}(0, 1)$.
4. Set new sample to: $x_{n+1} = \begin{cases} x' & \text{if } u < r, \\ x_n & \text{if } u \geq r. \end{cases}$

Some remarks:

- For a given target distribution p_* , a proposal distribution q is valid if $\text{supp}(p_*) \subset \cup_x \text{supp}(q(\cdot|x))$, i.e. $\forall x'$ with $p_*(x') > 0 \exists x$ s.t. $q(x'|x) > 0$.
- If q is symmetric, i.e. $q(x'|x) = q(x|x')$, then MH simplifies to the Metropolis algorithm with $\alpha = \frac{\tilde{p}(x')}{\tilde{p}(x)}$. Hastings made the correction for asymmetric q .

Analysis of MH Algorithm

We analyze with convergence of the MH algorithm:

1. MH generates a Markov chain with the transition kernel:

$$\pi(x'|x) = \begin{cases} q(x'|x)r(x'|x) & \text{if } x' \neq x, \\ q(x|x) + \sum_{x' \neq x} q(x'|x)(1 - r(x'|x)) & \text{if } x' = x. \end{cases}$$

$r(x'|x)$ is the conditional probability that x' is accepted after being proposed. We will show that the Markov chain satisfies the detailed balance condition:

$$p_*(x)\pi(x'|x) = p_*(x')\pi(x|x').$$

2. Let two states x and x' ($x \neq x'$) be arbitrarily fixed. Either

$$p_*(x)\pi(x'|x) \leq p_*(x')\pi(x|x'), \quad (\dagger)$$

or the reversed inequality holds. Without loss of generality, we proceed with inequality (\dagger) .

Analysis of MH Algorithm (cont'd)

$$p_*(x)\pi(x'|x) \leq p_*(x')\pi(x|x'). \quad (\dagger)$$

3. $(\dagger) \Rightarrow \alpha(x'|x) = \frac{p_*(x')q(x|x')}{p_*(x)q(x'|x)} \leq 1 \Rightarrow r(x'|x) = \alpha(x'|x)$
 $\Rightarrow \pi(x'|x) = q(x'|x)r(x'|x) = q(x'|x)\frac{p_*(x')q(x|x')}{p_*(x)q(x'|x)} = \frac{p_*(x')}{p_*(x)}q(x|x').$

4. $(\dagger) \Rightarrow \alpha(x|x') = \frac{p_*(x)q(x'|x)}{p_*(x')q(x|x')} \geq 1 \Rightarrow r(x|x') = 1$
 $\Rightarrow \pi(x|x') = q(x|x')r(x|x') = q(x|x').$

5. Combining (3) and (4), we conclude that $p_*(x)\pi(x'|x) = p_*(x')\pi(x|x')$.
Hence, by Theorem 1, p_* is a stationary distribution for the Markov chain.

6. If in addition the Markov chain generated by the MH algorithm is irreducible and aperiodic, then by Theorem 2 the Markov chain converges to the unique stationary distribution p_* .

Gibbs Sampling

Gibbs sampling:

Input: unnormalized target distribution $\tilde{p}((x_i)_{i \in \mathcal{V}})$, initial sample x^0 .

Loop $n \in \{0, 1, 2, \dots\}$, $i \in \mathcal{V}$:

Sample $x_i^{n+1} \sim p(x_i | x_{\{0, \dots, i-1\}}^{n+1}, x_{\{i+1, \dots, |\mathcal{V}|\}}^n)$.

Some remarks:

- If p is represented by a graphical model (i.e. BN or MRF), then sampling of x_i^{n+1} only involves the Markov blanket of i .
- Gibbs sampling can be interpreted as the MH algorithm with the proposal:

$$q(x'|x) = \delta_{x_{\mathcal{V} \setminus \{i\}}} (x'_{\mathcal{V} \setminus \{i\}}) p(x'_i | x_{\mathcal{V} \setminus \{i\}}),$$

and 100% acceptance rate:

$$\alpha = \frac{p(x')q(x|x')}{p(x)q(x'|x)} = \frac{p(x'_i | x'_{\mathcal{V} \setminus \{i\}}) p(x'_{\mathcal{V} \setminus \{i\}}) \delta_{x_{\mathcal{V} \setminus \{i\}}} (x'_{\mathcal{V} \setminus \{i\}}) p(x_i | x'_{\mathcal{V} \setminus \{i\}})}{p(x_i | x_{\mathcal{V} \setminus \{i\}}) p(x_{\mathcal{V} \setminus \{i\}}) p(x'_i | x_{\mathcal{V} \setminus \{i\}})} = 1.$$

Example: Gibbs Sampling for Pairwise CRF

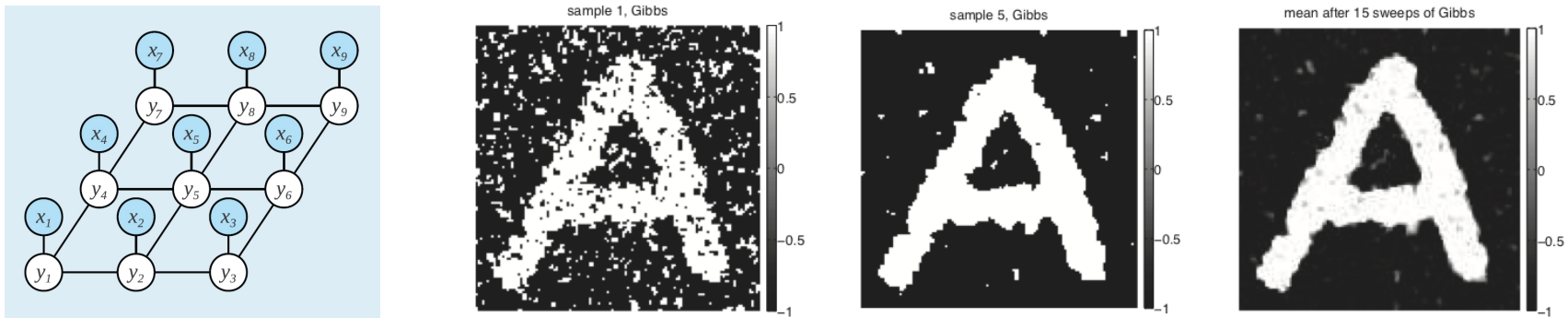


Figure: Gibbs Sampling for Pairwise CRF⁷.

We can apply Gibbs sampling to find

$$y \sim p(y|x) \propto \exp \left(- \sum_{i \in \mathcal{V}} E_i(y_i; x_i) - \sum_{(i,j) \in \mathcal{E}} E_{ij}(y_i, y_j) \right).$$

For each $i \in \mathcal{V}$, sample (e.g. by inverse CDF method):

$$y_i^{n+1} \sim p(y_i | x_i, y_{\text{nbr}(i)}^n) \propto \exp \left(- E_i(y_i) - \sum_{j \in \text{nbr}(i)} E_{ij}(y_i, y_j^n) \right).$$

⁷Sampled images taken from [Murphy, Figure 24.1].
 PGM SS19 : III : Inference on Graphical Models



Further Reading

- Murphy, Chapters 23, 24.
- Nowozin & Lampert, Sections 3.4.
- Koller & Friedman, Chapter 12.