

Markov chain Monte Carlo methods

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We want to approximate complex integral: let $x_1, \dots, x_N \sim p(x)$, then for any test function $h(x)$:

$$\mathbb{E}_{X \sim p}[h(X)] = \int h(x)p(x)dx \approx \frac{1}{N} \sum_{n=1}^N h(x_n).$$

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Here, x can be parameters or any latent variables of interest.

Importance sampling

Instead of sampling from p (hard to do because Z is unknown), sample $x \sim q$ and adjust for the difference between γ and q :

$$\int h(x)p(x)dx \approx \sum \bar{w}(x)h(x),$$

where $w(x) = \gamma(x)/q(x)$ and $\bar{w}(x) = w(x)/\sum_n w(x)$.

Sequential Monte Carlo methods

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- $x_d^n \sim q_d(x_d | x_{1:d-1})$.

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If $x = (x_1, \dots, x_D)$ is high-dimensional, we can sample each component sequentially:

- $x_d^n \sim q_d(x_d | x_{1:d-1})$.
- Interleave resampling step to maintain particle diversity and prune unpromising particles.

Sequential Monte Carlo methods

SMC methods work well when there is a temporal structure in x , where it is natural to sample one dimension at a time.

Sequential Monte Carlo methods

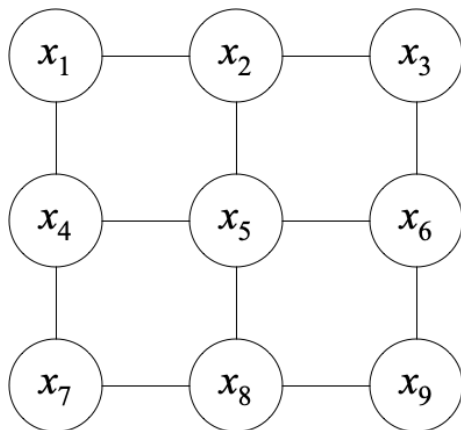
SMC methods work well when there is a temporal structure in x , where it is natural to sample one dimension at a time.

So why do we need another algorithm/method?

- Large variance associated with choice of proposal distribution.
- Curse of dimensionality may still manifest and approximation can be poor.

Example: Lattice

Consider a $K \times K$ 2-dimensional lattice $G = (V, E)$.



Example: Lattice

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- Image processing: Each node represents a pixel of an image. $X_v \in \{\text{black, white}\}$ or gray scale $X_v \in [0, 1]$ or RGB color.

Example: Ising model

Let $X = (X_v)$. The “energy” function for the Ising model is defined as:

$$H(x) = \sum_v \phi(x_v) + \sum_{(u,v) \in E} \psi(x_u, x_v),$$

- $(u, v) \in E$ denote neighbors (adjacent nodes),
- ϕ : unary potential,
- ψ : pairwise potential (measuring interaction strength).

Example: $\phi(x_v) = \beta x_v$ and $\psi(x_u, x_v) = \kappa x_u x_v$ for $\beta, \kappa \in \mathbb{R}$.

Example: Ising model

The probability distribution on X is defined as,

$$p(x) = \frac{1}{Z} \exp(-H(x))$$

where

$$Z = \sum_{x_v: v \in V} \exp(-H(x)).$$

Z in statistical physics is referred to as “partition function”. Essentially a normalization constant.

SMC for Ising model?

- Not obvious what order to sample the variables.
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- Not obvious what order to sample the variables.
- It could lead to very few unique values for x_v sampled earlier in the SMC iteration.
- Leads to poor approximation involving those sampled earlier on.
- For the Ising model, maybe it makes more sense to continually sample new values for x_v given x_{-v} until we are satisfied.

Metropolis-Hastings algorithm

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- Compute acceptance probability:

$$A(x'|x) = \min \left(1, \frac{\gamma(x')}{\gamma(x_{t-1})} \frac{q(x_{t-1}|x')}{q(x'|x_{t-1})} \right).$$

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- Sample $u \sim U(0, 1)$
- Set,

$$x_t = \begin{cases} x' & \text{if } u < A \\ x_{t-1} & \text{otherwise} \end{cases}$$

Why does MH work?

- If we take samples x_1, \dots, x_N using MH algorithm, why is this equivalent to taking samples from the target distribution $p(x)$?

Markov chain

Markov chain $\{X_t\}$ is a stochastic process modeling a sequence of events where the probability of each event depends only on the previous event.

- Markov property: $p(x_t | x_{1:t-1}) = p(x_t | x_{t-1})$.

Markov chain

Given measurable space $(\mathcal{X}, \mathcal{F})$,

$$K : \mathcal{X} \times \mathcal{F} \rightarrow [0, 1]$$

is referred to as the Markov kernel (a probability measure).

- Each random variable $X_t \in \mathcal{X}$
- $K(x, A)$ specifies the probability of moving to a set $F \in \mathcal{F}$ given that the chain is in state $x \in \mathcal{X}$.

Markov chain: continuous state space

For continuous state space, $\mathcal{X} = \mathbb{R}$, the transition probability can be described using a density function $K(x_{t-1}, x_t) = k(x_t|x_{t-1})$.

Markov chain: discrete state space

For discrete state space, the Markov chain is described using a transition matrix P , where P_{ij} represents the probability of transitioning from state i to state j , $P(x_t = j | x_{t-1} = i)$.

Markov chain: stationary distribution

The Markov chain $\{X_t\}$ converges to unique **stationary** distribution as $t \rightarrow \infty$ if some conditions are satisfied.

A probability distribution π defined on \mathcal{X} is invariant (stationary) under a Markov kernel K if for all $F \in \mathcal{F}$

$$\pi(A) = \int \pi(x)K(x, F)dx.$$

For discrete case: $\pi = \pi P$.

Markov chain: detailed balance (reversibility)

A Markov chain with kernel $K : \mathcal{X} \times \mathcal{F}$ satisfies the detailed balance condition with respect to a probability distribution π if,

$$\pi(x)k(x'|x) = \pi(x')k(x|x').$$

Reversibility: probability of being in state x and moving to x' from x is the same as being in state x' and moving to x .

- Note: detailed balance is a stronger condition than stationary condition: if detailed balance is satisfied, π is a stationary distribution of the Markov chain with kernel K .

Markov chain: Ergodicity

- 1 Aperiodic: Markov chain does not return to the same state at some fixed interval.
- 2 Positive recurrent: the expected number of steps for returning to the same state is finite.

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Claim: MH algorithm constructs a Markov chain on \mathcal{X} whose stationary distribution is $p(x)$.

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Markov transition kernel:

- given current state x , we move to a new state x' with probability

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- given current state x , we move to a new state x' with probability

$$q(x'|x)A(x'|x)$$

- stay at current state x with probability

$$q(x|x) + q(x'|x)(1 - A(x)).$$

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Case 1: $A(x'|x) = \frac{p(x')q(x|x')}{p(x)q(x'|x)} < 1$.

$$p(x)q(x'|x)A(x'|x) = p(x)q(x'|x)\frac{p(x')q(x|x')}{p(x)q(x'|x)} \quad (1)$$

$$= p(x')q(x|x'). \quad (2)$$

MH satisfies detailed balance

Case 2: $A(x'|x) \geq 1$.

$$p(x')q(x|x')A(x|x') = p(x')q(x|x') \frac{p(x)q(x'|x)}{p(x')q(x|x')} \quad (3)$$

$$= p(x)q(x'|x). \quad (4)$$

Is MH an ergodic Markov chain?

Yes, as long as we choose our proposal carefully.

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- For discrete case, ensure $q(x'|x) > 0$ for all $x', x \in \mathcal{X}$.

Metropolis-Hastings algorithm

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- Independent Metropolis refers to the case where a global proposal is used $q(x'|x) = q(x')$, which can lead to high rejection rates (why?).
- Large global proposals tend to be rejected, causing the chain to get stuck at a point for long periods.

Gibbs sampling

Gibbs sampling is an MCMC algorithm, which is well suited for high-dimensional distributions where sampling directly from the joint distribution is difficult.

Gibbs sampling

- 1 Initialize x^0 .

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- 2 For $t = 1, \dots, T$:
 - Iterate over each variable x_i :
 - ▶ Sample $x_i^t \sim p(x_i | x_{-i}^t)$, where x_{-i} refers to all other variables except x_i .

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This means that each variable is sampled from its conditional distribution given the current values of all other variables.

Gibbs sampling is particularly effective when the conditional distributions $p(x_i | x_{-i})$ are easy to sample from.

Why does Gibbs sampling work?

Claim: Gibbs sampling can be viewed as a special case of the Metropolis-Hastings algorithm where the proposal distribution is always accepted.

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Since $q(x'|x) = p(x'_i|x_{-i})$ and $q(x|x') = p(x_i|x_{-i})$, the acceptance probability simplifies to 1.

Gibbs for Ising model

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

- Sample $x_v \sim p(x_v | x_{-v})$ for each $v \in V$.

Sample each variable in turn, conditioned on the values of all of the other variables.

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- Sample $x_v \sim p(x_v | x_{-v})$ for each $v \in V$.

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What does $p(x_v | x_{-v})$ look like?

Gibbs sampling for Ising model

$$p(x_v | x_{-v}) = \frac{p(x_v, x_{-v})}{\sum_{x'_v} p(x'_v, x_{-v})} \quad (5)$$

$$\propto \exp(-\phi(x_v) - \sum_{(u,v) \in E} \psi(x_u, x_v)). \quad (6)$$

Example: image denoising

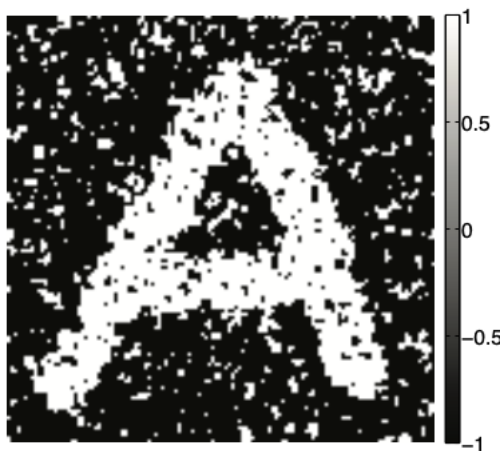


Figure 1: Fig 12.3 (a), PML 2

If all of the neighbors of x_v is white/black, x_v is likely to be white/black.

Example: image denoising

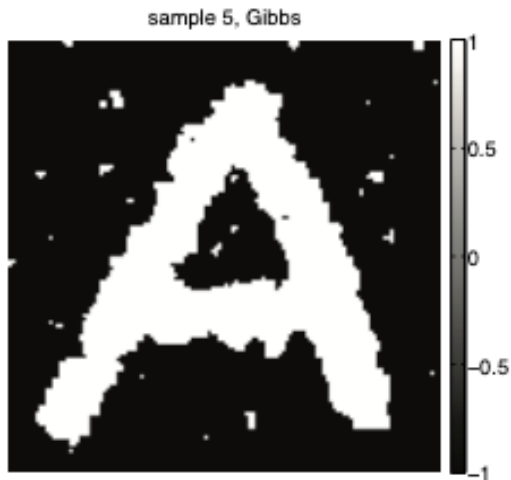


Figure 2: Fig 12.3 (b), PML 2

Example: image denoising

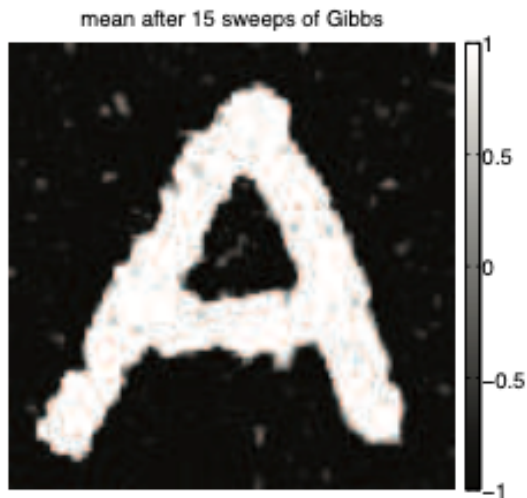


Figure 3: Fig 12.3 (c), PML 2

Undirected graphical models

Undirected graphical models (UGM):

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- Each node $v \in V$ represents a random variable.
- Edge between $u, v \in V$ is denoted (u, v) . Presence of an edge indicates that there is a symmetric relationship between u and v but we cannot easily pinpoint directionality.

Undirected graphical models

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- Commonly used for modeling dependence structure where directionality is unclear.
- Example: The value taken at each pixel (random variable X_v) is related to the value taken by its neighbors but it is not causal.

Undirected graphical models

- Pairwise Markov property: For any two non-adjacent nodes u, v ,
 $X_u \perp X_v \mid X_{rest}$.

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- Local Markov property: $X_u \perp X_{rest} \mid X_{nbr(u)}$, where $nbr(u) = \{v : (u, v) \in E\}$.

Undirected graphical models

- Pairwise Markov property: For any two non-adjacent nodes u, v , $X_u \perp X_v | X_{rest}$.
- Local Markov property: $X_u \perp X_{rest} | X_{nbr(u)}$, where $nbr(u) = \{v : (u, v) \in E\}$.
- Global Markov property:

Any two sets $A, B \subset V$, are conditionally independent given a separating set S , i.e., $X_A \perp X_B | X_S$, if S separates A and B in G .

Undirected graphical models

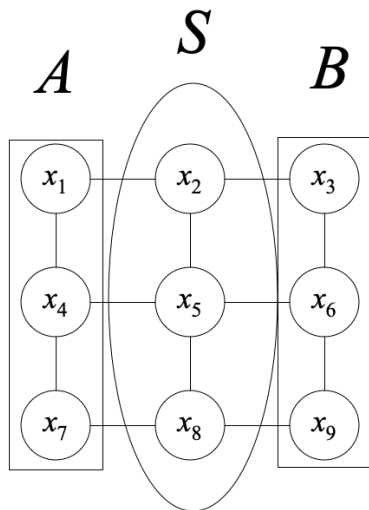


Figure 4: Global Markov property

Undirected graphical models

Markov blanket of v is defined as a minimal set of nodes that separates v from the rest of the nodes. It is given by, $MB(v) = nbr(v)$.

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MB plays a central role in determining efficient inference algorithm.
Example, Gibbs sampling update of a variable X_v is conditioned on its MB and nothing else.

Undirected graphical models

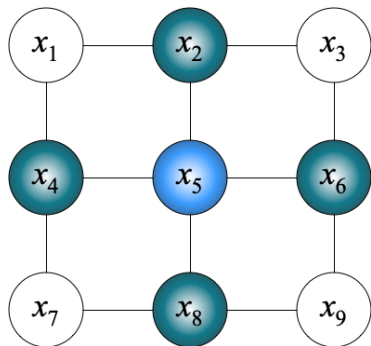


Figure 5: Markov blanket

Undirected graphical models: Hammersley-Clifford Theorem

A strictly positive probability distribution $p(x_V)$ satisfies the global Markov property with respect to G if and only if it can be factorized as,

$$p(x_V) = \frac{1}{Z} \prod_{C \in \mathcal{C}} \psi_C(x_C),$$

- \mathcal{C} denotes the set of (maximal) **cliques**,
- ψ_C denotes potential function for clique C ,
- Z is normalization constant also referred to as partition function.

Undirected graphical models

Clique $C \subseteq V$ of $G = (V, E)$ is a fully connected subgraph of G such that every pair of nodes $u, v \in C$ are adjacent i.e., $\{u, v\} \in E$.

A clique C is maximal if adding a node to C does not preserve full connectivity.

Undirected graphical models

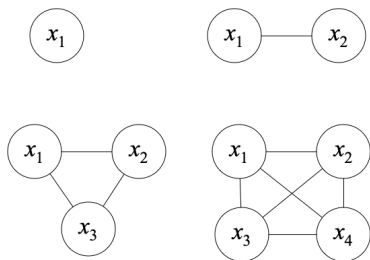


Figure 6: Example: Markov blanket

An edge $\{u, v\}$ is a clique. A fully connected set of nodes is a clique.

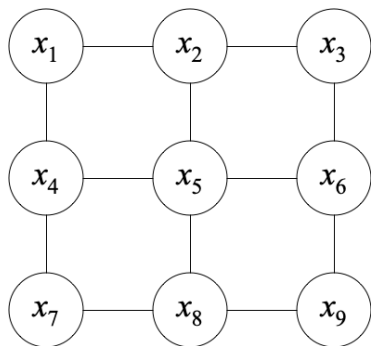
Undirected graphical models

Computing partition function is a source of great computational challenge:

$$Z = \int_{x_V} \prod_{C \in \mathcal{C}} \psi_C(x_C).$$

In most cases, the inference involving UGM requires approximate methods.

Undirected graphical models



What are the maximal cliques in this graph?

Back to Gibbs sampling

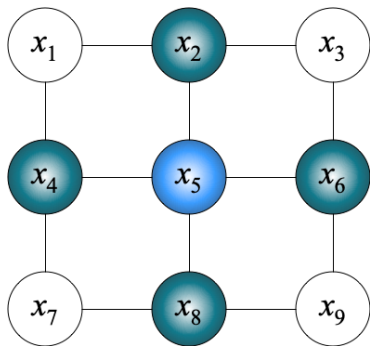
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Back to Gibbs sampling

Given an UGM, determine the Markov blanket for each node v .

Determine the conditional $p(x_v | x_{mb(v)})$.

Back to Gibbs sampling



Blocked Gibbs sampling

- Partition the nodes into disjoint sets $A, B \subset V$ such that

$$x_u \perp x_v | B, \quad u, v \in A$$

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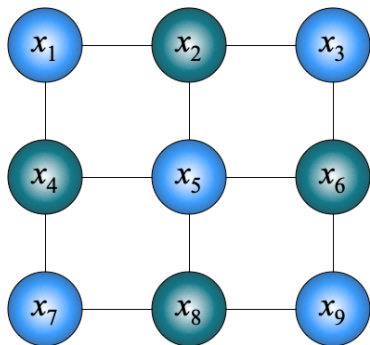
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$$x_u \perp x_v | A, \quad u, v \in B.$$

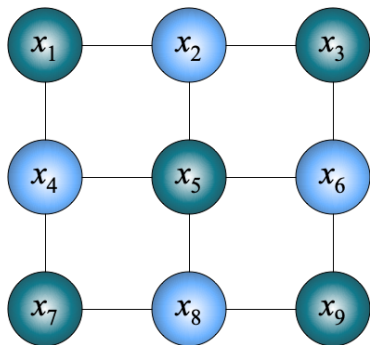
At each iteration $t = 1, \dots, T$:

- Sample $p(x_A | x_{-A})$,
- Sample $p(x_B | x_{-B})$.

Blocked Gibbs sampling



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- MCMC methods can be utilized to sample from intractable distributions.
- Metropolis-Hastings provides general sampling but requires careful proposal design for efficiency.
- Gibbs sampling is efficient when conditional distributions are easy to sample from, leveraging local dependencies.
- MRFs serve as a foundation for probabilistic inference, particularly in structured probabilistic models.

Applications of UGMs

- Neuroscience and associative memory: Hopfield networks (1982, 1984).
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 - ▶ Probabilistic generative models used in unsupervised pre-training of deep networks. Inspired contrastive divergence and other energy-based models in deep learning: the first “deep” neural network.
- Natural language processing and large language models (2017)
 - ▶ GPT-based large language models capture token dependencies.
 - ▶ The architecture is not a UGM (transformers use self-attention) but GPT learns long-range dependencies between tokens (subword) in non-sequential manner (not directional).