Readings: K&F 12.1, 12.2, 12.3, 12.4

Approximate | Inference I

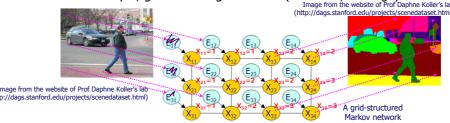
Lecture 15 – May 16, 2011 CSE 515, Statistical Methods, Spring 2011

Instructor: Su-In Lee

University of Washington, Seattle

Inference

- Inference is widely used,
 - Probabilistic queries: Given E=e, what is P(X E=e)?
 - For example, given E=image what is P(X=labels|E=image)=?



- Learning parameters with partially observed data
 EM, gradient ascent, etc
- but exact inference is expensive ←
 - O(Nn), where N=max_i|Val(C)|
 - Exponential blowup can be in N_i which for factor i can be v^m if factor i has m variables with v values each.

Approximate Inference Overview

Particle-based approximate inference

- Full particle methods
 - Sampling methods
 - Deterministic particle generation
- Distributional particles
- Applications & Simulation: data association

Global approximate inference

- Inference as optimization
- Generalized Belief Propagation
- Propagation with approximate messages
- Structured variational approximations

Particle-based Approximate Inference

General framework

- Generate particles (samples) x[1],...,x[M] from P
- Estimate function f by $\underbrace{E_{P}(f)}_{M}$
- For a function $f(X) = 1(Y = \hat{y})$
- P(Y=y) can be written as $E_P[f]$

.χ.

- How particles are generated?
 - Use forward sampling ←
 - Use likelihood weighting sampling ←

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5

Today...

Particle-Based Methods Overview

- Full particle methods
 - Sampling methods

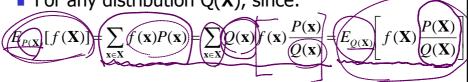


- Forward sampling, Likelihood weighting
- (Un-normalized/normalized) Importance sampling
- Markov chain Monte Carlo
- Deterministic particle generation
- Distributional particles

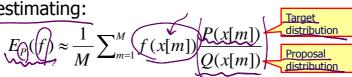
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Unnormalized Importance Sampling

For any distribution Q(X), since:



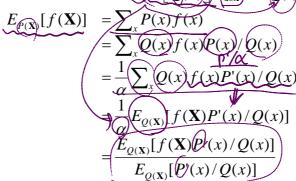
 We can estimate f(x) by generating samples from Q and estimating:



- Can show that estimator variance decreases with more samples M→∞
- Can show that Q=P is the lowest variance estimator

Normalized Importance Sampling

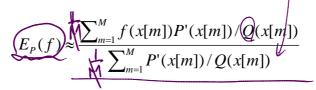
- Un-normalized importance sampling assumes known P
 - Usually we know P up to a constant $P = P/\alpha$, where $\alpha = \sum_{x} P'(x)$
 - Example: Posterior distribution P(X|E=e) = P(X|E=e) (a) where $\alpha = P(E=e)$
- We can estimate α by: $(P(\mathbf{X}))$ $(P(\mathbf{X}))$ (P
- Thus



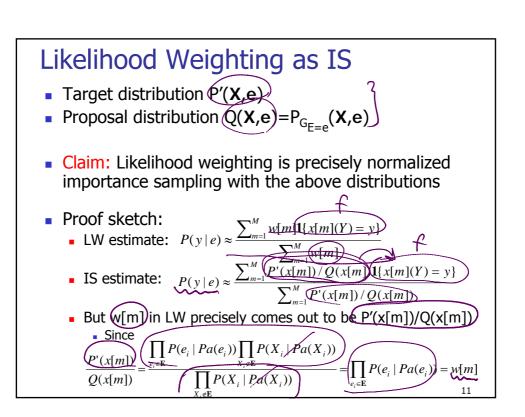
Normalized Importance Sampling

$$E_{P(\mathbf{X})}[f(\mathbf{X})] = \frac{E_{Q(\mathbf{X})}[f(\mathbf{X})P'(x)/Q(x)]}{E_{Q(\mathbf{X})}[P'(x)/Q(x)]}$$

Given M samples from Q, normalized sampling estimates function f by:



Importance Sampling for BayesNets Let's think about how to generate particles to estimate P(Y|e) Y6X P(Y|E=e) Define mutilated network G_{E=e} as: Nodes X∈E have no parents in G_{E=e} Nodes X∈E have CPD that is 1 for X=E[X] and 0 otherwise The parents and CPDs for all other variables are unchanged 0.6 0.7 0.3 Original Mutilated network G network G_{E=e} 0.1 Target distribution (P)(X) 0.4 0.99 0.01 Proposal distribution $Q(\mathbf{X},e) \neq P_{G_F}$



Particle-Based Methods Overview

- Full particle methods
 - Sampling methods
 - Forward sampling
 - Importance sampling



- Markov chain Monte Carlo (MCMC)
- Deterministic particle generation
- Distributional particles

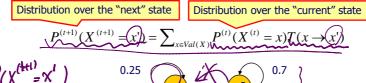
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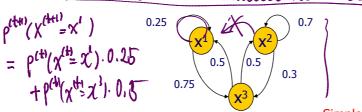
Markov Chain Monte Carlo

- Limitations of importance sampling
 - An evidence node affects the sampling only for nodes that are its descendants.
 - The effect on nodes that are non-descendants is accounted for only by the weights w's.
 - What if much of the evidence is at the leaves of the network?
 - We are essentially sampling from the prior distribution P(X), which
 is often very far from the desired posterio(P(X|E=e))
 - → Decreases the accuracy of the estimates
- An alternative sampling approach (MCMC)
 - General idea: Define a sampling process that is guaranteed to converge to taking samples from the posterior distribution of interest P(X|E=e)
 - Generate samples from the sampling process
 - Estimate f(X) from the samples.

Markov Chains

- A Markov chain consists of
 - A state space(Val(X))
 - Transition probability $T(x\rightarrow x')$ of going from state x to x'
- Distribution over subsequent states is defined as





Simple Markov chain

Stationary Distribution

$$P^{(t+1)}(X^{(t+1)} = x') = \sum_{x \in Val(X)} P^{(t)}(X^{(t)} = x) T(x \to x')$$

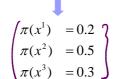
■ A distribution (x(X)) is a stationary distribution for a Markov chain T if it satisfies

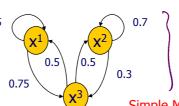
$$\pi(X = x') = \sum_{x \in Val(X)} \pi(X = x) T(x \to x')$$

$$\pi(x^1) = 0.25\pi(x^1) + 0.5\pi(x^3)$$

$$\pi(x^2) = 0.7\pi(x^2) + 0.5\pi(x^3)$$

$$\pi(x^3) = 0.75\pi(x^1) + 0.3\pi(x^2)$$
 0.25





Simple Markov chain

Markov Chains & Stationary Dist.

A Markov chain is regular if there is k such that for every x, x'∈Val(X), the probability of getting from x to x' in exactly k steps is greater than zero

2-7/

- Theorem: A finite state Markov chain T has a unique stationary distribution if and only if it is regular
- Goal: Define a Markov chain whose stationary distribution is P(X|e)

16

Gibbs Sampling ←

States

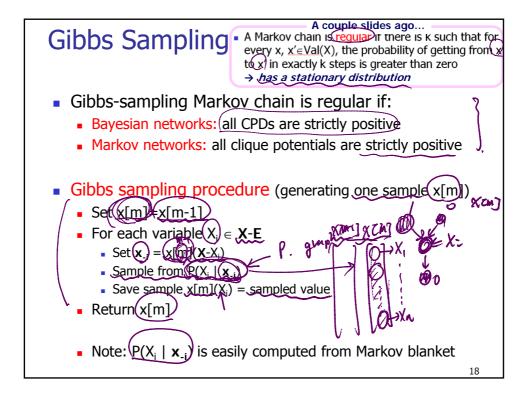
E=e

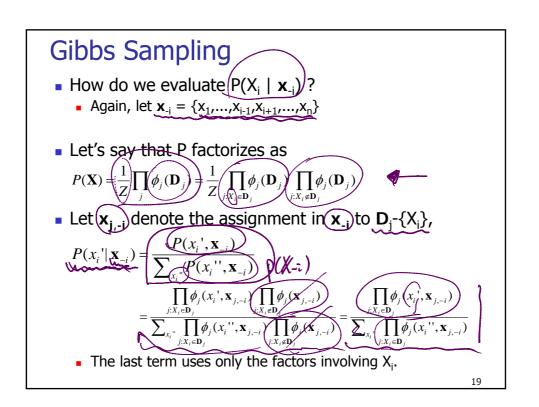
- Legal (=consistent with evidence) assignments to variables
- Transition probability

■ $T = T_1 \cdot ... \cdot T_k \leftarrow \chi_{\bar{\imath}}$

For each variable X_i , let (X_i) be (X_i) . Say that (X_i) = (X_i) . Say that (X_i) = (X_i) =

Claim: P(X|e) is a stationary distribution to the chain





Gibbs Sampling in Practice

- We need to wait until the burn-in time has ended number of steps until we take samples from the chain
 - We want to wait until the sampling distribution is close to the stationary distribution, P(1/e)
 - Hard to provide bounds in general for this 'mixing time'
 - Once the burn-in time ended, all samples are from the stationary distribution

 XCWD
- Note: after the burn-in time, samples are correlated. Consecutive samples from the same trajectory are correlated.
- Since no theoretical guarantees exist application of Markov chains is somewhat of an art
 - We can evaluate burn-in time by comparing the estimates $\hat{E}_k(f) \approx \left(\frac{1}{M} \sum_{m=1}^M f(x^k[m], e)\right)$ from multiple chains 1,...,

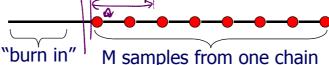
20

Sampling Strategy

- How do we collect the samples?
- Strategy I:
 - Run the chain M times, each run for N steps
 - Each run starts from a different state
 - Return the last state in each run

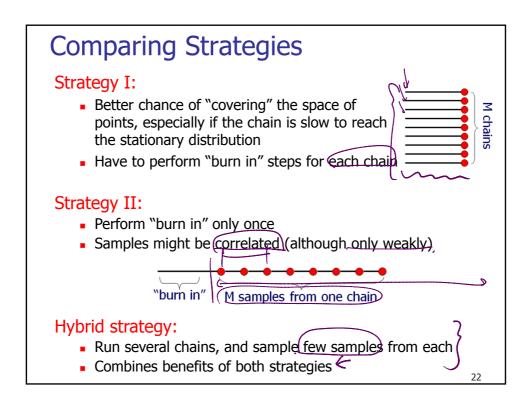


- Run one chain for a long time
- After some "burn in" period, sample points every some fixed number of steps



21

M chains



Particle-Based Methods Overview

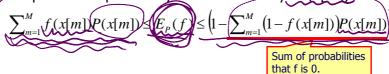
- Full particle methods
 - Sampling methods
 - Forward sampling
 - Importance sampling
 - Markov chain Monte Carlo
- ightharpoonup Deterministic particle generation \leftarrow
 - Distributional particles

Deterministic Search Methods

- Idea: if the distribution is dominated by a small set of instances, it suffices to consider only them for approximating the function
 - For instances that we generate(x[1],...x[M), estimate is



Note: we can obtain lower and upper bounds by examining the part of the probability mass covered by EP(x[m]).



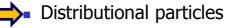
Key: how can we enumerate highly probably instantiations?

 Note: the single most probably instantiation is MPE which itself is an NP-hard problem

24

Particle-Based Methods Overview

- Full particle methods
 - Sampling methods
 - Forward sampling
 - Importance sampling
 - Markov chain Monte Carlo
 - Deterministic particle generation



- Until now, we discussed the cases where we are given particles that have full assignment of values on all variables.
- Can we use a partial assignment to estimate?

Distributional Particles

- Idea: use <u>partial assignments</u> to a subset of the network variables, combined with closed form representation of a <u>distribution</u> over the rest
 - \bullet (X_n) Variables whose assignments are defined by particles
 - •(X) Variables over which we maintain a distribution
 - Distributional particles are a.k.a Rao-Blackwellized particles
 - Estimation proceeds as

$$E_{P|e}(f) = \sum_{x_{p}, x_{d}} P(x_{p}, x_{d} | e) f(x_{p}, x_{d})$$

$$= \sum_{x_{p}} P(x_{p} | e) \sum_{x_{d}} P(x_{d} | x_{p}, e) f(x_{p}, x_{d})$$

$$= \sum_{x_{p}} P(x_{p} | e) E_{P(x_{p}|x_{p}, e)} [f(x_{p}, x_{d})])$$

- We can use any sampling procedure to sample X.
- We assume that we can compute the internal expectation efficiently

2

Distributional Particles

- Distributional particles define a continuum between
 - For $(|X_p|)=|X-p|$ we have full particles and thus full sampling
 - For $|X_p| = 0$ we are performing full exact inference



- Distributional Likelihood Weighting
 - Sample over a subset of the variables

$$P(y \mid e) \approx \frac{\sum_{m=1}^{M} w[m] \left(E_{P(X_d \mid x_p[m], e)} [\mathbf{1}\{x[m](y) = y\}] \right)}{\sum_{m=1}^{M} w[m]}$$

- Distributional Gibbs Sampling X_€ ←
 - Sample only a subset of the variables, transition probability is as before $\underline{T((\mathbf{u}_i, x_i) \to (\mathbf{u}_i, x_i'))} = P(x_i'|\mathbf{u}_i)$ but the computation may require inference

Broader Class of Markov Chains

- Limitations of Gibbs sampling
 - The Gibbs chain uses only very local moves over the state space: moves that chance only one variable at a time.
 - High-probability states will form strong basins of attraction, and the chain will be very unlikely to move away from such a state → the chain will mix very slowly.
 - We want to consider chains that allow a broader range of moves, including much larger steps in the space.
- Solutions
 - Block Gibbs sampling
 - Metropolis-Hastings algorithm

28

Block Gibbs Sampling

- There are cases where we can simultaneously sample several variables efficiently
- Block Gibbs algorithm
 - Assume that we can partition the variables X/into several disjoint blocks of variables X₁,...,X_i, such that we efficiently sample x_i from P(X) x₁,...,x_{i-1},x_{j+1},...,x_k)
 - Simple modification to Gibbs: Iteratively sample blocks of variables, rather than individual variables
 - It takes much "longer-range" transitions in the state space in a single sample step

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Metropolis-Hastings algorithm (1/3)

- Unlike the Gibbs chain, M-H algorithm does not assume that we can generate next-state samples from a particular target distribution
 - It uses the idea of a proposal distribution Q that we have already seen in the case of IS.

Basic ideas

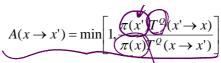
- We sample from a different distribution Q and then correct for the resulting error.
- However, unlike importance sampling, we do not want to keep track of importance weights.
 - They are going to decay exponentially with the number of transitions, leading to a whole slew of problems
- Instead, we randomly choose whether to accept the proposed transition, with a probability that corrects for the discrepancy between Q and the target distribution?

Metropolis-Hastings algorithm (2/3)

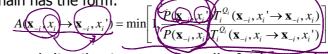
- Let our proposal distribution T9 define a transition model over our state space
 - For each state x To defines a distribution over possible successor states in Val(X), from which we select randomly a candidate next state x'
- We can either accept the proposal and transition to the new state x', or reject it and stay at x.
 - For each states (x, x') we have an acceptance probability $(A(x \to x'))$ Then, the actual transition model of the Markov chain is $T(x \to x') = T^{\varrho}(x \to x')A(x \to x') \qquad x \neq x'$ $T(x \to x) = T^{\varrho}(x \to x) + \sum_{x \neq x'} T^{\varrho}(x \to x')(1 A(x \to x'))$
 - We can show that with the following acceptance probabilities (and the regularity assumption), a chain I has the unique stationary distribution (proof in K&F page 516)

$$A(x \to x') = \min \left[1, \frac{\pi(x')T^{\mathcal{Q}}(x' \to x)}{\pi(x)T^{\mathcal{Q}}(x \to x')} \right]$$

Metropolis-Hastings algorithm (3/3)



- The M-H algorithm has a particularly natural implementation in the context of graphical models.
 - Each local transition mode T is defined via an associated proposal distribution T_i^o and the acceptance probability for this chain has the form:



- The proposal distributions are usually fairly simple, so it is easy to compute their ratios.
 - In the case of graphical models, the first ratio can also be computed easily:

npured easily: $\frac{P(\mathbf{x}_{-i}, x_i^{'})}{P(\mathbf{x}_{-i}, x_i^{'})} = P(x_i^{'} | \mathbf{x}_{-i})$ Similarly to Gibbs sampling, \mathbf{x}_i can be reduced to the Markov blanket of \mathbf{X}_i

32

So far, we discussed various sampling strategies. Let me talk about one example of real applications and "show" you how different sampling methods work in a toy model of the application.

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Application & Simulation: Data Association

Data association problem (aka correspondence problem)

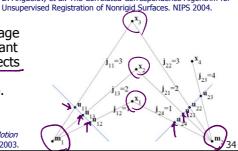
 Relating sensor measurements to parameters in the model that is being learned.

For example,

 We want to find a correspondence between a set of (automatically selected) landmarks on different 3D scans of human bodies.

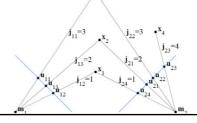
Given a set of image measurements **U**={u_{ik} for image i and measurement k}, we want to know which of the <u>3D objects</u> **X**={x_j, 1≤j≤n} each measurement corresponds to.

F. Dellaert, SM. Seitz, CE. Thorpe and S. Thrun. EM, MCMC, and Chain Flipping for Structure from Motion with Unknown Correspondence. Machine Learning 2003.



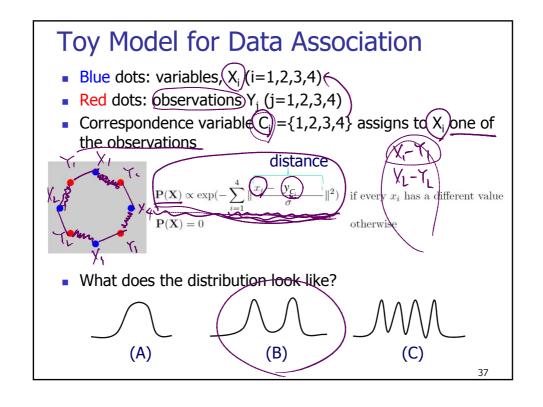
Application & Simulation: Data Association

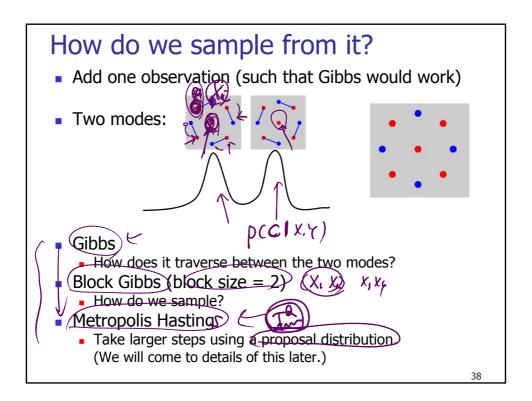
- Data association problem (aka correspondence problem)
 - Relating sensor measurements to parameters in the model that is being learned.
- Example problem
 - Given a set of image measurements U={u_{ik} for image i and measurement k}, we want to know which of the 3D objects X={x_j, 1≤j≤n} each measurement corresponds to.
 - To model the <u>correspondence between measurements up</u> and 3D object x_{ij} we introduce a correspondence vector **J**
 - For each measurement u_{ik}, the vector J contains an indicator variable j_{ik} indicating that u_{ik} is assigned to the j_{ik}-th object x.



F. Dellaert, SM. Seitz, CE. Thorpe and S. Thrun. EM, MCMC, and Chain Flipping for Structure from Motion with Unknown Correspondence. Machine Learning 2003.

Applications: Data Association ■ Maximize L(Θ; U) = ∑ L(Θ; U, J) ■ J's are hidden variables → EM algorithm ■ The E-step requires inference P(J| U, Θ(t)) ■ This problem has been tackled using range of models and a variety of inference methods including MCMC ■ Efficiency is important and we will "see" how various MCMC-based methods show varying performance ■ This problem has been tackled using range of models and a variety of inference methods including MCMC ■ Efficiency is important and we will "see" how various MCMC-based methods show varying performance ■ This problem has been tackled using range of models and a variety of inference methods including MCMC ■ Efficiency is important and we will "see" how various MCMC-based methods show varying performance ■ This problem has been tackled using range of models and a variety of inference methods including MCMC ■ Efficiency is important and we will "see" how various MCMC-based methods show varying performance





Let's "See" How They Work

Run the following Matlab scripts:

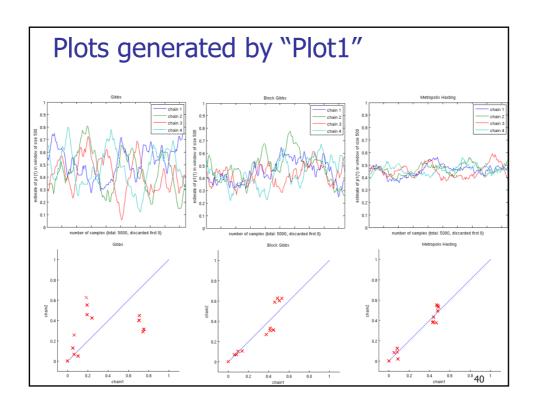
VisualMCMC1(10000, 0.1, 0.05);

% live animation of sampling

% parameters: num of samples, sigma, pause time after each sample

Plot1;

% the first few lines of Plot1.m contain the parameters you may want to play around with



Acknowledgement

- The MCMC sampler shown in class was written by Huayan Wang (Stanford, CS).
- These lecture slides were generated based on the slides from Prof Eran Segal and Huanyan Wang.

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