

Probabilistic Graphical Models

Approximate Inference: Parallel MCMC





Recap of MCMC



- Markov Chain Monte Carlo methods use adaptive proposals Q(x'|x) to sample from the true distribution P(x)
- Metropolis-Hastings allows you to specify any proposal Q(x'|x)
 - But choosing a good Q(x'|x) requires care
- Gibbs sampling sets the proposal Q(x'|x) to the conditional distribution P(x'|x)
 - Acceptance rate always 1!



Parallel MCMC for Large Scales

- Datasets and models can be very large
 - Millions to billions of data points
 - Millions to billions of random variables
 - Compute time measured in CPU-years
 - Need GBs to TBs of memory
 - E.x. Yahoo web graph has ~1.4 billion nodes and 6.6 billion edges
 - Imagine doing a Markov Random Field on that network
- Without parallelism, we cannot use large datasets and models!
 - Today: how to use multiple CPUs and machines in MCMC

Taking Multiple Chains

- Proper use of MCMC actually requires parallelism
 - To determine convergence, you need to take multiple MCMC chains
 - Chains are independent, so you can run one chain per CPU
 - Once converged, you can combine samples from all chains





Taking Multiple Chains

- Taking multiple chains doesn't solve all issues, though
 - If burn-in is long, then all chains will take a long time to converge!
 - We need a way to take each sample faster...



Idea: Run Gibbs Sampling in Parallel?





t	В	Е	Α	J	Μ
0	F	F	F	F	F
1					
2					
3					
4					

- Recall the alarm network
 - Initialize all variables at t = 0 to False
 - Idea: parallel Gibbs sample all variables at step t conditioned on t-1





t	В	Е	Α	J	Μ
0	F	F	F	F	F
1	F				
2					
3					
4					

• Sampling P(B|A,E) at t = 1: Using Bayes Rule, $P(B \mid A, E) \propto P(A \mid B, E)P(B)$

• (A,E) = (F,F), so we compute the following, and sample B = F $P(B = T | A = F, E = F) \propto (0.06)(0.01) = 0.0006$ $P(B = F | A = F, E = F) \propto (0.999)(0.999) = 0.9980$





t	В	Е	Α	J	Μ
0	F	F	F	F	F
1	F	Т			
2					
3					
4					

• Sampling P(E|A,B): Using Bayes Rule,

 $P(E \mid A, B) \propto P(A \mid B, E)P(E)$

• (A,B) = (F,F), so we compute the following, and sample E = T $P(E = T | A = F, B = F) \propto (0.71)(0.02) = 0.0142$ $P(E = F | A = F, B = F) \propto (0.999)(0.998) = 0.9970$





t	В	Е	Α	J	Μ
0	F	F	F	F	F
1	F	Т			
2					
3					
4					

- Notice the difference
 - Normal Gibbs sampling: compute P(E|A,B) based on B_{t=1}, A_{t=0}
 - Naïve Parallel GS: compute P(E|A,B) based on $B_{t=0}$, $A_{t=0}$
 - At step t, always condition on t-1 instead of most recently sampled value





t	В	Е	Α	J	Μ
0	F	F	F	F	F
1	F	Т	F		
2					
3					
4					

• Sampling P(A|B,E,J,M): Using Bayes Rule,

 $P(A \mid B, E, J, M) \propto P(J \mid A)P(M \mid A)P(A \mid B, E)$

• (B,E,J,M) = (F,F,F,F), so we compute the following, and sample A = F $P(A = T | B = F, E = F, J = F, M = F) \propto (0.1)(0.3)(0.001) = 0.00003$ $P(A = F | B = F, E = F, J = F, M = F) \propto (0.95)(0.99)(0.999) = 0.9396$





t	В	Е	Α	J	Μ
0	F	F	F	F	F
1	F	Т	F	Т	
2					
3					
4					

- Sampling P(J|A): No need to apply Bayes Rule
- A = F, so we compute the following, and sample J = T $P(J = T | A = F) \propto 0.05$ $P(J = F | A = F) \propto 0.95$





t	В	Е	Α	J	Μ
0	F	F	F	F	F
1	F	Т	F	Т	F
2					
3					
4					

- Sampling P(M|A): No need to apply Bayes Rule
- A = F, so we compute the following, and sample M = F $P(M = T | A = F) \propto 0.01$

$$P(M = F \mid A = F) \propto 0.99$$





t	В	Е	Α	J	Μ
0	F	F	F	F	F
1	F	Т	F	Т	F
2					
3					
4					

- We just finished sampling variables t=1
- Why is the sampling parallelizable?
 - We only conditioned on variable state at t=0, which is known in advance!
 - We can sample B,E,A,J,M on separate processors, without having to send information between processors



• E.g. collapsed Gibbs Sampling for LDA

$$P(z_i=j|\mathbf{z}_{-i},\mathbf{w}) \propto rac{n^{(w_i)}_{-i,j}+eta}{n^{(\cdot)}_{-i,j}+Weta}rac{n^{(d_i)}_{-i,j}+lpha}{n^{(d_i)}_{-i,\cdot}+Tlpha}$$

- Just assign different z_i 's to different processors or machines
- But there's a problem...

- Naïve Parallel GS may not converge to the stationary distribution
- Consider the following Bayes Net:



- Essentially an XOR relation between (A,B) and (A,C)
- Joint distribution P(A,B,C) has only 8 states, so we can compute the stationary distribution. It is dominated by 2 equally-probable states:
 - (A,B,C) = (T,F,T) and (A,B,C) = (F,T,F)





 Let's initialize (A,B,C) = (F,F,F) and see what happens when we naively Gibbs sample in parallel...





t	Α	В	С
0	F	F	F
1	Т		
2			
3			
4			

• Sampling P(A|B,C):

 $P(A | B, C) \propto P(B | A)P(C | A)$

• (B,C) = (F,F) so we sample A = T

 $P(A = T \mid B = F, C = F) \propto (0.999)(0.999) \approx 1$ $P(A = F \mid B = F, C = F) \propto (0.001)(0.001) \approx 0$





t	Α	В	С
0	F	F	F
1	Т	Т	
2			
3			
4			

- Sampling P(B|A): No need to apply Bayes Rule
- A = F so we sample B = T

$$P(B = T \mid A = F) \propto (0.999) \approx 1$$
$$P(B = F \mid A = F) \propto (0.001) \approx 0$$





t	Α	В	С
0	F	F	F
1	Т	Т	Т
2			
3			
4			

- Sampling P(C|A): No need to apply Bayes Rule
- A = F so we sample C = T

$$P(C = T \mid A = F) \propto (0.999) \approx 1$$
$$P(C = F \mid A = F) \propto (0.001) \approx 0$$





t	Α	В	С
0	F	F	F
1	Т	Т	Т
2	F	F	F
3			
4			

• Easy to see that at t=2, we will get (A,B,C) = (F,F,F)





t	Α	В	С
0	F	F	F
1	Т	Т	Т
2	F	F	F
3	Т	Т	Т
4			

- Easy to see that at t=2, we will get (A,B,C) = (F,F,F)
- At t=3, (A,B,C) = (T,T,T)





t	Α	В	С
0	F	F	F
1	Т	Т	Т
2	F	F	F
3	Т	Т	Т
4	F	F	F

- Easy to see that at t=2, we will get (A,B,C) = (F,F,F)
- At t=3, (A,B,C) = (T,T,T)
- At t=4, (A,B,C) = (F,F,F)





t	Α	В	С
0	F	F	F
1	Т	Т	Т
2	F	F	F
3	Т	Т	Т
4	F	F	F

- Easy to see that at t=2, we will get (A,B,C) = (F,F,F)
- At t=3, (A,B,C) = (T,T,T)
- At t=4, (A,B,C) = (F,F,F)
- Can you see the problem?

- We know the stationary distribution is [(F,T,F), (T,F,T)]
 - But naïve parallel GS gets stuck in [(T,T,T), (F,F,F)]



- Naïve parallel GS performs poorly on near-discrete distributions
- What is the correct way to Gibbs sample in parallel?



- Recall that in MRFs, we Gibbs sample by sampling from P(x| MB(x)), the conditional distribution of x given its Markov Blanket MB(x)
 - For MRFs, the Markov Blanket of x is just its neighbors
 - In the MRF below, the red node's Markov Blanket consists of the blue nodes





- Observe that we can *correctly* Gibbs sample the two green nodes simultaneously
 - Neither node is part of the other's Markov Blanket, so their conditional distributions do not depend on each other
 - Sampling one of the green nodes doesn't change the conditional distribution of the other node!





- How do we generalize this idea to the whole graph?
 - Find subsets of nodes, such that all nodes in a given subset are not in each other's Markov Blankets, and the subsets cover the whole graph
 - The subsets should be as large as possible
 - Because we can Gibbs sample all nodes in a subset at the same time
 - At the same time, we want as few subsets as possible
 - The Markov Blankets of different subsets overlap, so they cannot be sampled at the same time. We must process the subsets sequentially.





- We can find these covering subsets with k-coloring algorithms (Gonzales et al., 2011)
 - A k-coloring algorithm colors a graph using k colors, such that:
 - Every node gets one color
 - No edge has two nodes of the same color
- Trees always admit a 2-coloring (e.g. below)
 - Assign one color to some node, and alternate colors as you move away



- Bipartite graphs are always 2-colorable
 - Color each side of the bipartite graph with opposite colors
 - e.x. Latent Dirichlet Allocation model is bipartite
- However, not all graphs have k-colorings for all $k \ge 2$
 - In the worst case, a graph with n nodes can require n colors
 - The full clique is one such graph
 - Determining if a graph is k-colorable for k > 2 is NP-complete
 - In practice, we employ heuristics to find k-colorings
- Instead of using k-colorings, why not just Gibbs sample all variables at the same time?
 - The Markov Chain may become non-ergodic, and is no longer guaranteed to converge to the stationary distribution!

Online Parallel MCMC



- In "online" algorithms, we need to process new data points one-at-a-time
 - Moreover, we have to "forget" older data points because memory is finite
- For such applications to be viable, we can only afford constant time work per new data point
 - Otherwise we will reach a point where new data can no longer be processed in a reasonable amount of time
- We also want the algorithm to be parallel for scaling up
- What MCMC techniques can we use to make an online parallel algorithm?

Sequential Monte Carlo



- SMC is a generalization of Particle Filters
 - Recall that PFs incrementally sample $P(X_t|Y_{1:t})$, where the Xs are latent r.v.s and the Ys are observations under a state-space model
 - SMC does not assume the GM is a state-space model, or has any particular structure at all
- Suppose we have n r.v.s x_1, \ldots, x_n
 - SMC first draws samples from the marginal distribution $P(x_1)$, then $P(x_{1:2})$, and so on until $P(x_{1:n})$
 - Key idea: Construct proposals such that we sample from P(x_{1:k+1}) in constant time, given samples from P(x_{1:k})
 - Like other MCMC algorithms, we only require that we can evaluate $P'(x_{1:n}) = aP(x_{1:n})$ for some unknown a



- SIS is the foundation of Sequential Monte Carlo
 - It allows new variables to be sampled in constant time, without resampling older variables
- SIS uses proposal distributions with the following structure:

$$q_n(x_{1:n}) = q_{n-1}(x_{1:n-1})q_n(x_n \mid x_{1:n-1})$$
$$= q_1(x_1)\prod_{k=2}^n q_k(x_k \mid x_{1:k-1})$$

Notice we can propose x_{k+1} if we've already drawn x_{1:k}, without having to redraw x_{1:k}

• In normalized importance sampling, recall how the sample weights wⁱ are defined:

$$\langle f(X) \rangle_{P} = \sum_{i} f(x^{i}) w^{i}$$

where $w^{i} = \frac{r^{i}}{\sum_{i} r^{j}}$ and $r^{i} = \frac{P'(x^{i})}{Q(x^{i})}$

• In SIS, the unnormalized weights r can be rewritten as a telescoping product:

$$r(x_{1:n}) = \frac{P'_n(x_{1:n})}{q_n(x_{1:n})}$$

= $\frac{P'_{n-1}(x_{1:n-1})}{q_{n-1}(x_{1:n-1})} \frac{P'_n(x_{1:n})}{P'_{n-1}(x_{1:n-1})q_n(x_n | x_{1:n-1})}$
= $r_{n-1}(x_{1:n-1})\alpha_n(x_{1:n})$
= $r_1(x_1) \prod_{k=2}^n \alpha_k(x_{1:k})$

where

$$\alpha_n(x_{1:n}) = \frac{P'_n(x_{1:n})}{P'_{n-1}(x_{1:n-1})q_n(x_n \mid x_{1:n-1})}$$



$$r(x_{1:n}) = r_1(x_1) \prod_{k=2}^n \alpha_k(x_{1:k}) \quad \text{where} \quad \alpha_n(x_{1:n}) = \frac{P'_n(x_{1:n})}{P'_{n-1}(x_{1:n-1})q_n(x_n \mid x_{1:n-1})}$$

- This means the unnormalized weights r can be computed incrementally
 - Compute α_n and use it to update $r(x_{1:n-1})$ to $r(x_{1:n})$
 - NB: For this update to be constant time, we also require P'_n(x_{1:n}) to be computable from P'_{n-1}(x_{1:n-1}) in constant time
 - We remember the unnormalized weights r at each iteration, and compute the normalized weights w as needed from r
- Thus, we can sample x AND compute the normalized weights w using constant time per new variable x_n
 - So SIS meets the requirements for an online inference algorithm!
- Even better, the samples don't depend on each other
 - Assign one CPU core per sample to make the SIS algorithm parallel!



- SIS algorithm:
 - At time n = 1
 - Parallel draw samples $x_1^i \sim q_1(x_1)$
 - Parallel compute unnormalized weights $r_1^i = P_1'(x_1^i) / q_1(x_1^i)$
 - Compute normalized weights wⁱ₁ by normalizing rⁱ₁
 - Although this step is sequential, it takes almost no time to perform
 - At time $n \ge 2$
 - Parallel draw samples $x_n^i \sim q_n(x_n | x_{1:n-1}^i)$
 - Parallel compute unnorm. wgts. $r_n^i = r_{n-1}^i \alpha_n(x_{1:n}^i) = r_{n-1}^i \frac{P_n'(x_{1:n}^i)}{P_{n-1}'(x_{1:n-1}^i)q_n(x_n^i \mid x_{1:n-1}^i)}$
 - Compute normalized weights wⁱ_n by normalizing rⁱ_n
 - Although this step is sequential, it takes almost no time to perform



- But we are not done yet!
- Unfortunately, SIS suffers from a severe drawback: the variance of the samples increases exponentially with n!
 - See eq (31) of Doucet's SMC tutorial for an example
- Resampling at each iteration will decrease the sample variance!
 - Similar to weighted resampling from the first MC lecture!
Multinomial Resampling

- Suppose we have m samples x¹,...,x^m with corresponding importance weights w¹,...,w^m
- Construct a categorical distribution from these samples:
 - This distribution has m categories (choices)
 - The probability of drawing category k is w^k
 - Drawing category k gets us x^k
- To resample, just draw N times from this distribution
 - Note that N can be greater/less than m!
- For more advanced strategies such as systematic and residual resampling, refer to page 13 of Doucet's SMC tutorial

Why Resample?



- Apart from decreasing variance, there are other reasons...
- Resampling removes samples x^k with low weights w^k
 - Low-weight samples come from low-probability regions of P(x)
 - We want to focus computation on high-probability regions of P(x)
 - Notice that each sample gets an equal amount of computation, regardless of its weight w_k
 - Resampling ensures that more computation is spent on samples \boldsymbol{x}_k that come from high-probability regions of $\mathsf{P}(\boldsymbol{x})$
- Resampling prevents a small number of samples x_k from dominating the empirical distribution
 - Resampling resets all weights w_k to 1/N
 - This prevents sample weights w_k from growing until they reach 1

Sequential Monte Carlo

- The SMC algorithm is just SIS with resampling:
 - At time n = 1
 - **Parallel** draw samples $x_1^i \sim q_1(x_1)$
 - Parallel compute unnormalized weights $r_1^i = P_1'(x_1^i) / q_1(x_1^i)$
 - Compute normalized weights wⁱ₁ by normalizing rⁱ₁
 - Parallel resample wⁱ₁, xⁱ₁ into N equally-weighted particles xⁱ₁
 - At time $n \ge 2$
 - Parallel draw samples $x_n^i \sim q_n(x_n | x_{1:n-1}^i)$
 - Parallel compute unnorm. wgts. $r_n^i = r_{n-1}^i \alpha_n(x_{1:n}^i) = r_{n-1}^i \frac{P'_n(x_{1:n}^i)}{P'_{n-1}(x_{1:n-1}^i)q_n(x_n^i \mid x_{1:n-1}^i)}$
 - Compute normalized weights wⁱ_n by normalizing rⁱ_n
 - Parallel resample wⁱ_n,xⁱ_{1:n} into N equally-weighted particles xⁱ_{1:n}



Summary

• Parallel Gibbs sampling

- Naïve strategy: sample all variables at the same time
- Correct strategy: perform graph colorings and sample same-colored nodes in parallel
- Sequential Monte Carlo
 - Uses incremental proposal distributions
 - Provides a framework for designing online, parallel MCMC algorithms

Parallel Inference for Bayesian Nonparametric

- Dirichlet Process Mixture Model (recap)
- Inference schemes (recap)
- Parallel inference schemes
- Results



People sit on the table with the most preferred dish/color



- Table:
 - Cluster
- People:
 - Items to be clustered
- Parameters:
 - Dish/color on each table
 - Center of each cluster
- Hidden Variable:
 - Assignment of people to each table



People sit on the table with the most preferred dish/color



Which clustering algorithm will it lead to?



People sit on the table with the most preferred dish/color



Which clustering algorithm will it lead to?

Hard Kmeans



People sit on the table proportional to appreciation of dish/color



Which clustering algorithm will it lead to?



People sit on the table proportional to appreciation of dish/color



Which clustering algorithm will it lead to?

Soft Kmeans



Soft Kmeans Generative Model



appreciation of dish/color



People sit on the table proportional to appreciation of dish/color and number of people sitting on the table



Which clustering algorithm will it lead to?

Dirichlet Distribution Mixture Model





People sit on the table proportional to appreciation of dish/color and number of people sitting on the table



Which clustering algorithm will it lead to?

Dirichlet Distribution Mixture Model



People sit on the table proportional to appreciation of dish/color and number of people sitting on the table





People sit on the table proportional to appreciation of dish/color and number of people sitting on the table



Turning the definition





Stick Breaking Construction





Stick Breaking Construction



Graphical Model Representation Proportional to Which table each number of customer customer sit at sitting on the table V. Z_n 1. Draw $V_i \mid \alpha \sim \text{Beta}(1, \alpha), \quad i = \{1, 2, ...\}$ α 2. Draw $\eta_i^* | G_0 \sim G_0, \quad i = \{1, 2, \ldots\}$ 3. For the *n*th data point: Xn λ (a) Draw $Z_n | \{v_1, v_2, \ldots\} \sim \operatorname{Mult}(\pi(\mathbf{v})).$ (b) Draw $X_n | z_n \sim p(x_n | \eta_{z_n}^*)$. Ν ∞ **Dirichlet Process Mixture** Model Which dish is selected at each

table



- Gibbs Sampling:-
 - Sample each of the variable given the rest.
 - Variables to sample are table proportion V_k , table assignment to each customer (Z) and dish at each table η





- Gibbs Sampling:-
 - Sample each of the variable given the rest.
 - Variables to sample are table proportion V_k , table assignment to each customer (Z) and dish at each table η
 - Parallel inference: Easy





• Gibbs Sampling:-

- Sample each of the variable given the rest.
- Variables to sample are table proportion V_k , table assignment to each customer (Z) and dish at each table η
- Parallel inference: Easy
- Poor mixing



- Collapsed Gibbs Sampler:-
 - Integrate out V_k and η_k
 - Leads to better mixing
 - Parallel inference: Hard





Collapsed Gibbs suffer from large computational cost



Time (minutes)

• Variational Inference

- Approximate the posterior with a distribution belonging to a more manageable family of distribution
- Parallel inference: Easy
- Search within a restricted class of models, looses the expressiveness
- Typically less accuracy than MCMC methods



• Sequential Monte Carlo Method:-

- Keep a pools of particles, approximate the distribution using weighted combination of the pool
- Parallel inference: Easy
- High variance for naïve implementation, needs resampling (MCMC)



• Naïve

- Run collapsed sampler on individual core
- Combine the result approximately !!





• Naïve

- Run collapsed sampler on individual core
- Combine the result approximately !!
 - How
 - Why should two newly discovered clustered in two different processor be the same?



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- Idea: Dirichlet Mixture of Dirichlet processes are Dirichlet
 processes
- Skeptic(proof coming)



Idea: Dirichlet Mixture of Dirichlet processes are Dirichlet processes



Restaurant 1

 $D_j \sim \mathsf{DP}\left(\frac{\alpha}{P}, H\right), \quad j = 1, \dots, P$





Idea: Dirichlet Mixture of Dirichlet processes are Dirichlet processes





Idea: Dirichlet Mixture of Dirichlet processes are Dirichlet processes



Auxiliary Variable Model For DP

• The generative process is as follows :-

Proof



• If $G \sim DP(\alpha, G_0)$ and $\theta_1 \sim G$ Then posterior distribution is given by: $\theta_{n+1}|\theta_1, \dots, \theta_n \sim \sum_{l=1}^n \frac{1}{n+\alpha} \delta_{\theta_l} + \frac{\alpha}{n+\alpha} G_0$

• If $D_j \sim DP(\alpha/P, G_0), \phi \sim Dir(\frac{\alpha}{P}, \dots, \frac{\alpha}{P}), \pi_i \sim \phi$ and $\theta_i \sim D_{\phi_i}$, Then

$$\theta_{n+1}|\theta_1, \dots, \theta_n \sim \sum_{j=1}^P P(\pi_{n+1} = j | \pi_1, \dots, \pi_n)$$

$$P(\theta_{n+1}| \pi_{n+1} = j, \pi_1, \dots, \pi_n, \theta_1, \dots, \theta_n, G_0)$$

$$= \sum_j \frac{n_j + \alpha/P}{n - 1 + \alpha}$$

$$\left\{ \sum_{l=1}^n \frac{1}{n_j + \alpha/P} \delta_{\theta_l} \delta_{\pi_l = j} + \frac{\alpha/P}{n_j + \alpha/P} G_0 \right\}$$

$$= \sum_{l=1}^n \frac{1}{n + \alpha} \delta_{\theta_l} + \frac{\alpha}{n + \alpha} G_0$$



- Conditioned on the Restaurant allocation data are distributed according to P independent Dirichlet process
- Perform local collapsed gibbs sampling on the independent DPs
- For the global parameters perform MH
 - Select a cluster 'c' and a processor 'p'
 - Propose: move 'c' to 'p'
 - Acceptance ratio depends on cluster size
- Can pass the indices of the cluster item.
- Can be done asynchronously without affecting the performance.

Result





Extension to HDP



Take home message



- Naïve parallel inference scheme does not always work
- Utilize structure of the problem: Conditional independence
- Exact parallel inference or bound on error