

Probabilistic Graphical Models

Approximate Inference: Parallel MCMC



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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



- If burn-in is long, then all chains will take a long time to converge!
- We need a way to take each sample faster...



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Idea: Run Gibbs Sampling in Parallel?





t	В	Ε	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 $P(B = T \mid A = F, E = F) \propto (0.06)(0.01) = 0.0006$ $P(B = F \mid A = F, E = F) \propto (0.999)(0.999) = 0.9980$





t	Β	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 $P(E = T \mid A = F, B = F) \propto (0.71)(0.02) = 0.0142$ $P(E = F \mid A = F, B = F) \propto (0.999)(0.998) = 0.9970$





t	В	Ε	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





• 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	Ε	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 $P(J = T \mid A = F) \propto 0.05$ $P(J = F \mid A = F) \propto 0.95$





t	B	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 $P(M = T \mid A = F) \propto 0.01$ $P(M = F \mid A = F) \propto 0.99$





t	В	Ε	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

- In practice, works very well for some graphical models
 - E.g.
 - collapsed Gibbs Sampling for LDA

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

- Asynchronous Distributed Learning of Topic Models, Arthur Asuncion, Padhraic Smyth, Max Welling
- Distributed Algorithms for Topic Models, David Newman, Arthur Asuncion, Padhraic Smyth, Max Welling
- 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):

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

• (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 x₁,...,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:

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

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

ere

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

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

- 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 x_k that come from high-probability regions of P(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}

-Scalable Dynamic Nonparametric Bayesian Models of Content and Users, Amr Ahmed and Eric Xing

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}

-Scalable Dynamic Nonparametric Bayesian Models of Content and Users, Amr Ahmed and Eric Xing

Asynchronous Sequential Monte Carlo

- Use a cascade of particles
- Barrier synchronization
- Shown to be consistent and unbiased estimate

-Asynchronous Anytime Sequential Monte Carlo, Brooks Paige, Frank Wood, Arnaud Doucet and Yee Whye The, NIPS 2014



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





 $\theta \sim Dir(\alpha)$ for i=1, ... N $Z_i \sim Mul(\theta)$ $X_i \sim f(\eta_{zi})$



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 Which table each customer sit at



- 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



- Finding scientific topics, Thomas L. Griffiths and Mark Steyvers PNAS 2004

- Parallel Gibbs Sampling 1:-
 - Sample V_k and n_k globally
 - Given V_k and n_k , Z are independent of each other



- Parallel Gibbs Sampling:-
 - Sample V_k and n_k globally
 - Given V_k and n_k , Z are independent of each other
 - Poor mixing



- Parallel Gibbs Sampling 2:-
 - Sample V_k and n_k globally
 - Sample a noisy version of V_k and n_k for each processor
 - Sample Z independently in each processor



-Distributed Algorithms for Topic Models, David Newman, Arthur Asuncion, Padhraic Smyth, Max Welling

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





Collapsed Gibbs suffer from large computational cost



• 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 !!





0

• 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?



• Naïve

- Sample Hyper parameter for each
- Run collapsed sampler on individual core





- Asynchronous Distributed Learning of Topic Models, Arthur Asuncion, Padhraic Smyth, Max Welling, NIPS 2009

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Idea: Dirichlet Mixture of Dirichlet processes are Dirichlet
processes



Idea: Dirichlet Mixture of Dirichlet processes are Dirichlet
processes



Restaurant 1

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


Parallel MCMC



Idea: Dirichlet Mixture of Dirichlet processes are Dirichlet processes



Parallel MCMC



Idea: Dirichlet Mixture of Dirichlet processes are Dirichlet processes



Auxiliary Variable Model For DP

• The generative process is as follows :-

Inference

- 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





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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