Quantum Annealing for Dirichlet Process Mixture Models with Applications to Network Clustering

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Abstract

We developed a new quantum annealing (QA) algorithm for Dirichlet process mixture (DPM) models based on the Chinese restaurant process (CRP). QA is a parallelized extension of simulated annealing (SA), i.e., it is a parallel stochastic optimization technique. Existing approaches [Kurihara et al. 2009; Sato et al. 2009] cannot be applied to the CRP because their QA framework is formulated using a fixed number of mixture components. The proposed QA algorithm can handle an unfixed number of classes in mixture models. We applied QA to a DPM model for clustering vertices in a network where a CRP seating arrangement indicates a network partition. A multi core processor was used for running QA in experiments, the results of which show that QA is better than SA, Markov chain Monte Carlo inference, and beam search at finding a maximum a posteriori estimation of a seating arrangement in the CRP. Since our QA algorithm is as easy as to implement the SA algorithm, it is suitable for a wide range of applications.

Keywords: Quantum annealing, Dirichlet process, Stochastic optimization, Maximum a posteriori estimation, Bayesian nonparametrics

1. Introduction

Clustering is one of the most important topics in machine learning because it is a fundamental approach to analyze differences and similarities of data. In statistical machine learning, a probabilistic latent variable model is used for clustering. The Dirichlet process mixture (DPM) models [Antoniak 1974] are well studied and they enable us to handle an unfixed number of classes, which means that we do not have to decide the number of classes in advance. In other words, they can estimate the number of classes according to data. A DPM model is often represented by the Chinese restaurant process (CRP) [Aldous 1985], in which clustering is represented as a seating arrangement of customers in a restaurant. This representation is a useful one helping us understand the clustering process in DPM models.

A clustering problem using a probabilistic model is generally formulated as a maximum a posteriori (MAP) estimation in statistical machine learning. Since finding the exact MAP solution will be difficult in many cases, we have to search for an approximate one. Markov chain Monte Carlo (MCMC) inference is widely used for the CRP [Neal 2000] but the MCMC is not necessarily appropriate for the MAP estimation. When we use MCMC for the MAP estimation, we extract a single class assignment with the highest probability in the class assignments sampled from the posterior distribution. The problem is that this sampling distribution (i.e., the posterior distribution) has to be stationary, and much iteration is needed before it converges.

DaumeIII (2007) showed that a beam search provides an attractive alternative to the MCMC in the CRP and another approach for the MAP estimation is a stochastic search. One of the most well-known stochastic search algorithms is simulated annealing (SA) [Kirkpatrick et al. 1983], which is similar to the MCMC but has an additional parameter, called a temperature, controlling the uncertainty of the search space. SA is known to find the global optimum when the cooling temperature reduction...
Figure 1: The left-hand panel shows the running of SA, in which \( \sigma \) indicates a seating arrangement of \( N \) customers in the CRP (i.e., a class assignment of \( N \) data points). The right-hand panel shows QA, in which multiple SAs interact through \( f \). \( \sigma_j \) indicates a seating arrangement of the CRP running in the \( j \)-th process. Note in QA that \( \sigma_m \) is interacted with \( \sigma_{m-1} \) and \( \sigma_1 \) (i.e., \( \sigma_{m+1} = \sigma_1 \)), which is mathematically derived from the QA framework (Theorem 53). During iterations, we control the hyper-parameters.

In this work, we focus on a novel stochastic search algorithm, quantum annealing (QA), which has attracted attention as an alternative annealing method for optimization problems in quantum information science. QA has been shown experimentally converge faster than to find better local optimums for Ising spin models. It has a parameter inducing quantum fluctuation, so the search space is controlled in a way different from that in SA. The details are explained below.

QA is a parallelized extension of SA in which quantum fluctuation is induced by running multiple SAs with interactions. Let us consider running \( m \) SAs, and let \( \sigma_j \) \((j = 1, \ldots, m)\) indicate a state (e.g., a class assignment) of \( N \) data points in the \( j \)-th simulation. In the CRP, we formulate \( \sigma_j \) as a table-seating arrangement of customers in the \( j \)-th CRP (see Fig. 1). We denote \( N \) data points as \( \mathbf{x} = (x_1, x_2, \ldots, x_N) \). The log-likelihood model given \( \sigma_j \) (i.e., \( \log p(\mathbf{x}, \sigma_j) \)) is based on the way the data is modeled. For simplicity, we denote the log-likelihood by \( \log p(\sigma_j) \). In this work, we use the Newman model for clustering network data (explained in Sec. 7). QA runs multiple dependent SAs with dependent here meaning that there is interaction \( f \) among neighboring SAs (see right-hand panel in Fig. 1).

We describe QA in terms of an optimization problem. When we run \( m \) SAs with different random initializations independently, we optimize \( \log p(\sigma_j) \) individually. That is, we find \( \sigma_j^* = \arg \max_j \log p(\sigma_j) \) for each \( j \) and we choose \( \sigma \) that has the highest \( \log p(\sigma_j^*) \) of all \( j \). In QA, we optimize the joint probability of \( m \) CRPs’ states \( \{\sigma_j\}_{j=1}^m \):

\[
\max_{(\sigma_1, \sigma_2, \ldots, \sigma_m)} \log p_{QA}(\{\sigma_1, \sigma_2, \ldots, \sigma_m\}),
\]

where \( p_{QA}(\cdot) \) is a probability measure over a set of states, which means that each state \( \sigma_j \) \((j = 1, \ldots, m)\) can take an independent state and QA gives the probability for these states. A set of states \( (\sigma_1, \sigma_2, \ldots, \sigma_m) \) represents (quantum) superposition of different states. That is, \( p_{QA}(\cdot) \) is a probability measure over superposition of different states in the limit of \( m \to \infty \) in quantum physics. In the CRP, \( (\sigma_1, \sigma_2, \ldots, \sigma_m) \) represents a superposition of \( m \) seating arrangements. The optimization problem (1) is actually formulated as

\[
\max_{(\sigma_1, \sigma_2, \ldots, \sigma_m)} \sum_{j=1}^{m} \log p_{SA}(\sigma_j) + f \cdot R(\sigma_1, \sigma_2, \ldots, \sigma_m),
\]

where the first term corresponds to the summation over \( m \) SA objectives, and \( R(\cdot) \) is regarded as a regularizer among \( m \) states, which are described in Sec. 5. This optimization is derived from the QA framework explained in Sec. 3. QA was recently used for solving practical optimization problems, such as clustering and variational Bayes inference, and it outperformed SA. Figure 2 summarizes QA and related work.

**Problems:** Existing approaches cannot be applied to the CRP because they need a fixed number of mixture components. Moreover, these approaches have to use a heuristic such as purity to apply their QA algorithms to the clustering problem. Therefore, a different formulation is needed.

**Contributions:** The purpose of this study is to propose a QA algorithm for the CRP. The key point is how to represent the states of data in the CRP. The existing work represents the data states as “which class a data point is assigned to.” That is, they require \( K \)-dimensional indicator vectors to represent the data states, and \( K \) (the number of classes) is given and fixed. We instead represent the
states of data as “which data points a data point shares the table with” in the CRP. That is, we use an N-by-N bit matrix to represent the data states, and this matrix indicates a seating arrangement in the CRP and does not depend on \( K \). This bit-matrix representation of the CRP is a novel idea and a key point in applying QA to the CRP. Note that the bit matrix is only used for mathematically deriving QA for the CRP. We do not directly use the matrix in an actual algorithm, whereas the existing approaches directly use the similarity matrix for clustering data.

2. Chinese Restaurant Process (CRP)

The CRP is a distribution over partitions such as clustering and is composed of three elements: a customer, table, and restaurant. In a clustering problem, the customer denotes a data point and the table denotes a data class. A seating arrangement of customers in a restaurant indicates a class assignment of data. In QA, we run multiple CRPs, i.e., we consider the seating arrangements in multiple restaurants.

The CRP assigns a probability for the seating arrangement of the customers in which \( Z = \{z_i\}_{i=1}^N \) denotes the seating arrangement of the customers and \( z_i = k \) indicates that customer \( i \) sits at the \( k \)-th table. \( N \) indicates the number of customers. When customer \( i \) enters a restaurant with \( K \) occupied tables at which other customers are already seated, customer \( i \) sits at a table with the following probability:

\[
p(z_i | Z, z_i; \alpha) \propto \begin{cases}  
N_k - 1 & (k\text{-th occupied table}), \\
\alpha & (new\text{ unoccupied table}) 
\end{cases}
\]

where \( N_k \) denotes the number of customers sitting at the \( k \)-th table, and \( \alpha \) is the hyper parameter of the CRP. A customer tends to select a new table when \( \alpha \) takes large value.

The log-likelihood of \( Z \) is given by

\[
p(Z) = \frac{\alpha^{K(Z)}}{\prod_{i=1}^{N-1-i+\alpha}} \prod_{k=1}^{K(Z)} (N_k - 1)!, \quad \text{where } K(Z) \text{ is the number of occupied tables in } Z.
\]

3. Quantum Annealing for CRP

This section explains how we derive QA for the CRP (QACRP). First, we introduce some notations and explain QACRP intuitively. Second, we introduce a bit matrix to reformulate the CRP for using QA independent of the number of classes, which
the (c into account (Eq.(3)). The QACRP sampler derived in Eq.(4) introduces the effect of customers who share tables with customer 2 in the (j-1)-th and (j+1)-th CRPs. In this case, since customers 1, 3, and 4 are customers who share tables with customer 2 in the (j-1)-th and (j+1)-th CRPs, the 1st table in the j-th CRP has these “two” customers and so takes the effect $e^{-\beta f(\beta, \Gamma)}$ into account ($c_{j-1}^c(2) + c_{j+1}^c(2) = 2$ in Eq. (4)). That is, in the QACRP sampler, when interaction $f(\beta, \Gamma)$ is large, a customer tends to sit with customers sharing the table in other CRPs.

is a key idea in this work. Third, we formulate the CRP by using a “density matrix” that is a basic formulation in quantum mechanics. Finally, we apply the Suzuki-Trotter expansion (Trotter, 1959; Suzuki, 1976) to approximate QACRP because the first-derived QACRP is intractable because of the computational cost of a matrix exponential.

3.1. Main result (See Fig. 3 for an intuitive image)

QACRP uses multiple restaurants. $z_{j,i} = k$ indicates that customer $i$ sits at the $k$-th table in the $j$-th restaurant. $Z_j = \{z_{j,i}\}$ denotes the seating arrangements of customers in the $j$-th restaurant. $c_{j,k}^+(i)$ denotes the number of customers who sit at the $k$-th table in the $j$-th restaurant and share tables with customer $i$ in the $(j+1)$-th restaurant. $c_{j,k}^-(i)$ denotes the number of customers who sit at the $k$-th table in the $j$-th restaurant and share tables with customer $i$ in the $(j-1)$-th restaurant. Customer $i$ sits at a table in the $j$-th restaurant with the following probability:

$$p_{QA}(z_{j,i} | Z_d)^m \{z_{j,i} \; ; \beta, \Gamma\} \propto \begin{cases} \frac{N_{j,k}}{\alpha + N - 1} \alpha & \text{(k-th occupied table)}, \\ \frac{\alpha}{\alpha + N - 1} \beta & \text{(new unoccupied table)}, \end{cases}$$

(4)

where $N_{j,k}$ denotes the number of customers sitting at the $k$-th table in the $j$-th restaurant. $f(\beta, \Gamma)$ is derived in Sec.3.2 Eq.(17) where $\beta$ and $\Gamma$ are hyper parameters that are called inverse temperature and quantum effect, respectively. The inverse temperature is also the hyper parameter of SA. When you change the CRP in Eq.(3) into QACRP in Eq.(4), all you have to do is to count the customers sharing tables in neighboring CRPs and introduce $f(\beta, \Gamma)$. Figure 3 shows an example of QACRP and provides an intuitive explanation. When $f(\beta, \Gamma) = 0$, QACRP is equivalent to $m$ independent CRPs with inverse temperature $\beta/m$, which we call SACRPs. We provide the details of the derivation in the next sections.

3.2. Bit matrix representation for CRP

We represent seating arrangement $Z$ by using a bit matrix $B$ in order to reformulate the CRP without fixing the number of tables (see Contributions in Sec. 1). Although this bit matrix representation seems to have high computational complexity, in an actual algorithm of QA, we do not need the direct calculation to the bit matrix.

A bit matrix $B$ looks like an adjacency matrix of customers (see Fig. 3) and $B$ denotes an $N$-by-$N$ bit matrix where $B_i$ is the $i$-th row vector, i.e., $B_i = (B_{i,1}, B_{i,2}, \ldots, B_{i,N})$, and $B_{i,n}$ is the $i$-th row and the $n$-th column element of $B$ or the $n$-th element of $B_i$. $\tilde{\sigma}_{i,n}$ is a two-dimensional indicator vector, i.e., it takes $(1, 0)^\top$ or $(0, 1)^\top$. We correspond $B_{i,n} = 1$ to $\tilde{\sigma}_{i,n} = (1, 0)^\top$ and $B_{i,n} = 0$ to $\tilde{\sigma}_{i,n} = (0, 1)^\top$, which means we can represent $B$ by using the $2N^2$ dimensional indicator vector, $\sigma$, as follows:

$$B \Leftrightarrow \sigma = \bigotimes_{i=1}^{N} \bigotimes_{n=1}^{N} \tilde{\sigma}_{i,n}.$$

(5)

$\otimes$ is the Kronecker product, which is a special case of a tensor product. If $A$ is a $k$-by-$l$ matrix and $B$ is an $m$-by-$n$ matrix, then the Kronecker

\[...\]
product $A \otimes B$ is the following $km$-by-$ln$ block matrix:  
\[ A \otimes B = \begin{pmatrix} a_{11}B & \cdots & a_{1l}B \\ \vdots & \ddots & \vdots \\ a_{k1}B & \cdots & a_{kl}B \end{pmatrix}. \]
For example, $(1,0)^T \otimes (0,1)^T = (0,1,0,0)^T$. $\Sigma$ denotes a set of $\sigma_i$, i.e., $|\Sigma| = 2^{N^2}$.

The bit matrix $B$ is regarded as a seating arrangement as follows. If $B_{i,n} = 1$, the $i$-th and the $n$-th customers share a table. Note that we need the following conditional to represent seating arrangements with the bit matrix:

1. $B_{i,n} = B_{n,i}$ (symmetric matrix)
2. $B_{i,i} = 1 (i = 1, 2, \cdots, N)$, i.e., $\text{Tr } B = N$
3. $\forall i$ and $l$, $\frac{B_{i,n}}{B_{l,n}} = 1$ or $0$, where $\cdot$ is the inner product.

$\text{Tr } X$ is the trace of $X$. $\Sigma(\subset \Sigma)$ denotes a set of $\sigma$ corresponding to $B$ satisfying the above conditions. We call these conditions “seating conditions.”

Here, $\tilde{\delta}_i$ indicates the state of the $i$-th customer, i.e., with whom the $i$-th customer shares a table (see the left-hand side of Fig. 4) and $\tilde{\sigma}_i$ is a $(2N-1)$-dimensional indicator vector given by

\[ \tilde{\sigma}_i = \bigotimes_{n=1}^{i-1} \tilde{\delta}_{i,n} \otimes \bigotimes_{n=i+1}^N \tilde{\delta}_{i,n} \otimes \bigotimes_{n=1,n \neq i}^N \tilde{\delta}_{n,i}. \quad (6) \]

Let $\tilde{\Sigma}_i$ be a set of the states that $\tilde{\delta}_i$ can take under the seating conditions (i.e., $\sigma \in \Sigma$) when the $i$-th row elements and the $i$-th column elements are blank and the others are filled (see the right-hand side of Fig. 4). Since $\tilde{\Sigma}_i$ is a set of table-assignment states of the $i$-th customer, $|\tilde{\Sigma}_i| = K(Z \setminus \{z_i\}) + 1$. For example, the right-hand side of Fig. 4 shows table assignments of the 2nd customer when customers 1, 3, 4, and 5 have already been seated.

The right-hand side of Fig. 4 shows an example of $\tilde{\Sigma}$. Let $\tilde{\Sigma}$ be a set of table-assignment states of the 2nd customer when customers 1, 3, 4, and 5 have already been seated.

$\rho^{(2)}_{2N-1}$ is defined as a $2N-1$ dimensional indicator vector given by

\[ \rho^{(2)}_{2N-1} = \bigotimes_{n=1}^{i-1} (0,1)^T \otimes N \bigotimes_{n=i+1}^N (0,1)^T \bigotimes_{n=1,n \neq i}^N (0,1)^T. \quad (7) \]

The right-hand side of Fig. 4 shows an example of $\rho^{(2)}_{2N-1}$. We use $\rho^{(2)}_{2N-1}$ only in Appendix A.

### 3.3. Density matrix representation for classical CRP

We define the energy function $E$ over $\sigma^{(i)} \in \Sigma \ (i = 1, \cdots, 2^{N^2})$ by $E(\sigma^{(i)}) = -\log p(\sigma^{(i)})$, where if $\sigma^{(i)} \in \Sigma \setminus \tilde{\Sigma}$, then $p(\sigma^{(i)}) = 0$, i.e., $E(\sigma^{(i)}) = +\infty$.

The probability of a state $\sigma \in \Sigma$ is given by

\[ p(\sigma) = \frac{1}{Z} e^{-H_c \sigma}, \quad (8) \]

where $H_c = \text{diag} \left[ E(\sigma^{(1)}), E(\sigma^{(2)}), \cdots, E(\sigma^{(2^{N^2})}) \right]$, and $\text{diag}[]$ denotes a diagonal matrix. Note that $Z = \sum_{\sigma} e^{-H_c \sigma} = \text{Tr } e^{-H_c}$, where $H_c$ is called the classical Hamiltonian. If $\sigma \in \tilde{\Sigma}$, then $p(\sigma)$ is equal to $p(Z)$, i.e., $p(\sigma)$ is the probability over a seating arrangement. Since $H_c$ is diagonal, $e^{-H_c}$ is also diagonal with the $k$-th diagonal element $e^{-E(\sigma^{(k)})}$. That is, $p(\sigma^{(k)}) = \frac{1}{Z} e^{-E(\sigma^{(k)})}$.

### 3.4. Formulation for quantum CRP

The basic approach to expanding a classical system to a quantum one is to make the Hamiltonian
non-diagonal, i.e., add some off-diagonal elements while keeping hermiticity. We define a non-diagonal matrix $H$ by

$$H = H_c + H_q,$$

where $H_q$ is a non-diagonal matrix (we describe the definition of $H_q$ later). Intuitively, diagonal elements are filled with zero, and some off-

diagonal elements are filled with $\Gamma$ in $H_q$. That is, $H_c$ is given by $H_c$ and quantum effect $\Gamma$ is a basic approach in quantum physics and has also worked well in (Kurihara et al., 2009; Sato et al., 2009). The meaning of this formulation was described in (Sato et al., 2009) in terms of uncertainty.

The probability of a state $\sigma(\in \Sigma)$ in a quantum system is given by

$$p_{QA}(\sigma; \beta, \Gamma) = \frac{1}{Z} \sigma^\top e^{-\beta(H_c+H_q)} \sigma,$$

where $Z = \sum_\sigma \sigma^\top e^{-\beta(H_c+H_q)} \sigma = \text{Tr}[e^{-\beta(H_c+H_q)}]$.

The optimization problem

$$\max \sigma \log p_{QA}(\sigma; \beta, \Gamma)$$

could be solved by using the eigenvalue decomposition of the density matrix $e^{-\beta(H_c+H_q)}$, but, this approach is intractable because of its large computational cost.

One approximation approach for solving the optimization problem (11) is a stochastic search by drawing a state of the $i$-th customer, $\tilde{\sigma}_i$, from

$$p(\tilde{\sigma}_i | \sigma\tilde{\sigma}_i) = \frac{\sigma^\top e^{-H_c \sigma}}{\sum_{\tilde{\sigma}_i} \sigma^\top e^{-H_c \sigma}},$$

$$p_{QA}(\tilde{\sigma}_i | \sigma\tilde{\sigma}_i; \beta, \Gamma) = \frac{\sigma^\top e^{-\beta(H_c+H_q) \sigma}}{\sum_{\tilde{\sigma}_i} \sigma^\top e^{-\beta(H_c+H_q) \sigma}},$$

where $\sigma\tilde{\sigma}_i$ indicates that bits excluding the $i$-th row and the $i$-th column elements are standing. The summation over $\tilde{\sigma}_i$ is actually the summation of $\tilde{\sigma}_i \in \Sigma_i$; therefore, the classical expression $p(\tilde{\sigma}_i | \sigma\tilde{\sigma}_i)$ is tractable when $p(\tilde{\sigma}_i | \sigma\tilde{\sigma}_i)$ is another expression of Eq. (12). Calculation of the probability of the quantum system $p_{QA}(\tilde{\sigma}_i | \sigma\tilde{\sigma}_i; \beta, \Gamma)$, however, is intractable because of the exponential operation of a non-diagonal matrix $H = H_c + H_q$. We therefore need another approach described in Sec. 3.5.

We define $H_q$ as follows.

$$H_q = -\Gamma \sum_{i=1}^N \sum_{n=1}^N \sigma^\top_{i,n} E = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \sigma^\top = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$\sigma^\top_{i,n} = \left( \bigotimes_{t=1}^{i-1} E \right) \otimes \left( \bigotimes_{t=1}^{n-1} E \right) \otimes \sigma^\top \otimes \left( \bigotimes_{t=n+1}^{N} E \right) \otimes \left( \bigotimes_{t=1}^{N} E \right),$$

where $\Gamma$ is the quantum effect parameter. This formulation means that diagonal elements are filled with zeros, and some off-diagonal elements are filled with $\Gamma$ in $H_q$. Although other definitions can be considered, we define this formulation so that we can make the derivation of the search algorithm tractable by using an approximation method that is easy to implement.

3.5. Approximation inference for QACRP

We cannot calculate $p_{QA}(\tilde{\sigma}_i | \sigma\tilde{\sigma}_i; \beta, \Gamma)$ because $\sigma^\top e^{-\beta H} \sigma$ is intractable because of the non-diagonal matrix $H$. We use the Suzuki-Trotter expansion (Trotter, 1959; Suzuki, 1976) to approximate $p_{QA}(\tilde{\sigma}_i | \sigma\tilde{\sigma}_i; \beta, \Gamma)$.

We consider multiple running CRPs in which $\sigma_j(j = 1, \cdots, m)$ indicates the seating arrangement of the $j$-th CRP and represents the $j$-th bit matrix $B_j$. We correspond $B_{j,i,n} = 1$ to $\tilde{\sigma}_{j,i,n} = (1, 0)^T$ and $B_{j,i,n} = 0$ to $\tilde{\sigma}_{j,i,n} = (0, 1)^T$, which means that we can represent $B_j$ as $\sigma_j$ by using Eq. (13). We derive the following theorem:

Theorem 3.1. $p_{QA}(\sigma; \beta, \Gamma)$ in Eq. (10) is approximated by the Suzuki-Trotter expansion as follows:

$$p_{QA}(\sigma; \beta, \Gamma) = \frac{1}{Z} \sigma^\top e^{-\beta(H_c+H_q) \sigma} = \sum_{\sigma_j(j \geq 2)} p_{QA-ST}(\sigma, \sigma_2, \cdots, \sigma_m; \beta, \Gamma) + O\left(\frac{\beta^2}{m}\right),$$

(15)
where we rewrite $\sigma$ as $\sigma_1$, and

$$p_{QA-ST}(\sigma_1, \sigma_2, \ldots, \sigma_m; \beta, \Gamma) = \prod_{j=1}^{m} \frac{1}{Z(\beta, \Gamma)} e^{-\frac{2}{m}E(\sigma_j) + f(\beta, \Gamma)s(\sigma_j, \sigma_{j+1})},$$  \hspace{1cm} (16)$$

$$f(\beta, \Gamma) = 2 \log \coth \left( \frac{\beta}{m} \Gamma \right),$$  \hspace{1cm} (17)$$

$$s(\sigma_j, \sigma_{j+1}) = \sum_{i=1}^{N} \sum_{n=1}^{N} \delta(\sigma_{j+i, n}, \sigma_{j+1+i, n}),$$  \hspace{1cm} (18)$$

$$Z(\beta, \Gamma) = \left[ \sinh \left( \frac{\beta}{m} \Gamma \right) \right]^{2N} \sum_{\sigma} e^{-\frac{1}{2}E(\sigma)}.$$

Note that $\sigma_{m+1} = \sigma_1$. The proof is given in Appendix A. Note that our derived $f$ in Eq.(17) does not include the number of classes, $K$, whereas the $f$ in existing work [Kurihara et al. (2009); Sato et al. (2009)] is formulated by using a fixed $K$.

Equation (15) is interpreted as follows. $p_{QA}(\sigma; \beta, \Gamma)$ is approximated by marginalizing out other states $\{s_j\}_{j \geq 2}$ of $p_{QA-ST}(\sigma_1, \sigma_2, \ldots, \sigma_m; \beta, \Gamma)$. As shown in Eq.(16), $p_{QA-ST}(\sigma_1, \sigma_2, \ldots, \sigma_m; \beta, \Gamma)$ looks like the joint probability of the states of $m$ dependent CRPs. In Eq.(16), $e^{-\frac{2}{m}E(\sigma)}$ corresponds to the classical CRP with inverse temperature and $e^{f(\beta, \Gamma)}s(\sigma, \sigma_{j+1})$ indicates the quantum effect part. If $f(\beta, \Gamma) = 0$, which means CRPs are independent, $p_{QA-ST}(\sigma_1, \sigma_2, \ldots, \sigma_m; \beta, \Gamma)$ is equal to the products of probability of $m$ classical CRPs. $s(\sigma_j, \sigma_{j+1}) (> 0)$ is regarded as a similarity function between the $j$-th and $(j + 1)$-th bit matrices. If they are the same matrices, then $s(\sigma_j, \sigma_{j+1}) = N^2$. In Eq.(2), log $p_{QA}(\sigma_j)$ corresponds to $\log e^{-\frac{2}{m}E(\sigma_j)/Z}$ and the regularizer term $f \cdot R(\sigma_1, \ldots, \sigma_m)$ is $\log \prod_{j=1}^{m} e^{f(\beta, \Gamma)s(\sigma_j, \sigma_{j+1})} = f(\beta, \Gamma) \sum_{j=1}^{m} s(\sigma_j, \sigma_{j+1})$.

Note that we aim at deriving the approximation inference for $p_{QA}(\sigma, \beta; \Gamma)$ in Eq.(13). Using Theorem 3.1, we can derive Eq.(4) as the approximation inference. The details of the derivation are provided in Appendix B.

4. Experiments

We evaluated QA in a real application. We applied QA to a DPM model for clustering vertices in a network where a seating arrangement of the CRP indicates a network partition.
4.2. Dataset

We used three social network datasets, Netscience, Citeseer, and Wikivote. Netscience is a coauthorship network of scientists working on a network that has 1,589 scientists (vertices). Citeseer is a citation network dataset for 2,110 papers (vertices). Wikivote is a bipartite network constructed using administrator elections and vote history data in Wikipedia. Its 7,115 vertices represent Wikipedia users and a directed edge from vertex $i$ to vertex $j$ represents that user $i$ voted for user $j$. Netscience, Wikivote, and Citeseer respectively correspond to network examples a, b, and c in Fig. 5. We used the vertices in these networks to represent customers in the CRP, and we used a negative log-likelihood as an energy function to find the MAP solution.

4.3. Annealing schedule

We tested several $\beta/m$ schedules using combinations of $\beta_0 = 0.2m$, $0.4m$, and $0.6m$ and $\beta = \beta_0 \log(1 + t)$, $\beta_0 \sqrt{T}$, and $\beta_0 t$, where $t$ denotes the $t$-th iteration. The results we observed in our experiments showed that $\beta_0 = 0.4m$ and $\beta_0 \sqrt{T}$ created a better schedule in SA in terms of the MAP estimation. That is, $\beta$ increases to $\beta_0 \sqrt{T}$, where $T$ is the total number of iterations. In QA, we use the same $\beta/m$ schedule we used in SAs. Note that since the new table is easy to sample at very small $\beta$ (where the probability distribution becomes flat, see Eq. (4)), the SACRP has many tables at small $\beta$ and converges very slowly. That is, inverse temperatures that are too low do not work well in the CRP.

Since interaction $f$ is a function of $\Gamma$ and $\beta$, in practice we have to consider the schedule of $f(\beta, \Gamma)$. The interaction $f(\beta, \Gamma)$ increases when $\frac{\beta \Gamma}{m}$ decreases. QA is known to work well when $f(\beta, \Gamma)$ starts from zero (i.e., “independent” multiple SAs) and gradually increases. This process of $f(\beta, \Gamma)$ is achieved when $\frac{\beta \Gamma}{m}$ is a decreasing function of $t$. Therefore, we use

$$\frac{\beta \Gamma}{m} = \Gamma_0 \frac{T}{t},$$

where $\Gamma_0$ is a tuning parameter.

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1. [http://www.casos.cs.cmu.edu/computational_tools/datasets/external/netscience/](http://www.casos.cs.cmu.edu/computational_tools/datasets/external/netscience/)
2. [http://www.cs.umd.edu/projects/linqs/projects/ibc/index.html](http://www.cs.umd.edu/projects/linqs/projects/ibc/index.html)
3. [http://snap.stanford.edu/data/wiki-Vote.html](http://snap.stanford.edu/data/wiki-Vote.html)
4.4. Experimental settings

Our purpose is to search for a better MAP solution to a CRP in a small number of iterations (or short running time). We evaluated optimization algorithms in terms of maximum log-likelihood because we want a state with the highest log-likelihood. We compared QA with SA and the beam search. We used the beam search with an inadmissible score function that achieved the best performance in [Daume III, 2007]. We set the beam-width to 100. We did not compare the variational inference with QA because the variational inference cannot deal with the Chinese restaurant formation of the Dirichlet process mixture. That is, it is hard to compare them because their objective functions are different.

Since we used a multi core processor with 16 cores, we set $m = 16$ (i.e., ran one CRP at one core). We set $\alpha = 1$ in the CRP. $\alpha$ is easy to estimate in SAs and QA, but beam search cannot estimate it; therefore, we fixed it in these experiments. The number of iterations, $T$, for SAs and QA was 30. We generated 16 random seating arrangements $\{\sigma_{j}^{(\text{random})}\}_{j=1}^{16}$ for the initial settings of QA and 16 SAs, i.e., we use $\sigma_{j}^{(\text{random})}$ for the same initial setting of the $j$-th seating arrangement. Moreover, we compared QA ($m = 16$) with 1600 SAs where their MAP solutions are the best one of 1600 simulations with different random initializations. In 1600 SAs, we tried 100 seeds and generated $m = 16$ random seating arrangements for each seed, i.e., we ran the CRPs with $100 \times m = 1600$ initial seating arrangements.

4.5. Results and Discussions

Figure 6 shows the experimental results. QA and SAs outperformed the beam search because each line takes a positive value. QA finds a better local optimum than that of 16 and 1600 SAs at some $\Gamma_0$. This means that it is useful to run QA with changing $\Gamma_0$ rather than to run multiple SAs.

The effective $\Gamma_0$ has a positive correlation with the number of nodes. For example, the effective $\Gamma_0$ is around 2 in Netscience and is around 3.5 in Wikivote, which has more nodes than that of Netscience does. This is because the quantum effect term depends on $C \cdot f(\beta, \Gamma)$, where $C$ is the number of customers who share tables and thus depends on the number of customers (nodes). This means that the effective parameter range can be inferred from the number of nodes and we have only to check a few $\Gamma_0$ values.

QA needs more time and memory than SA with the linear order of $m$ because QA uses $m$ CRPs. However, when a parallel processing environment can be used and we run multiple SAs in parallel, the scalability of QA is the same as that of SAs. QA ($T = 30, m = 16$) and SA ($T = 30, m = 1$) took about 15 and 13 seconds for Netscience, about 25 and 22 seconds for Netscience, and about 79 and 76 seconds for Wikivote, where each value was the averaged running time of a single simulation for SA. Because of the multi core processing and the caching of customers sharing tables, the running time of QA was almost the same as that of a single SA. Therefore, QA makes the CRPs converge faster and finds a better seating arrangement than multiple-run SAs. The estimated number of classes achieving the best performance in QA ($m = 16$), 16 SAs, 1600 SAs and the beam search are 26, 22, 65, and 61 for Netscience, 37, 35, 30, and 57 for Citeseer, and 8, 8, 8, and 27 for Wikivote.

We found that a small $\Gamma_0$ induces a fast schedule of $f$, which means $f \gg 0$ at small $\beta$. The fast schedules make the convergence of QA too fast; therefore, QA converges to a worse optimum. QA is similar to SAs at large $\Gamma_0$ because interaction $f$ remains at almost 0 for a limited number of iterations. Larger $\Gamma_0$ makes CRPs in QA more independent, which means the results of QA approach those of SA. We found that interaction $f$ is almost zero when $\Gamma_0 = 5$ and $T = 30$, which means that the performance of QA is similar to that of SA. Therefore, in practice, we only check values of $\Gamma_0$ in descending order from a large value of $\Gamma_0$, such as $\Gamma_0 = 5$. That is, the effective value range is easy to infer from some $\Gamma_0$ values (in our experimental results, we show some non-effective values in order to provide the negative examples of QA).

5. Conclusion

We proposed a QA algorithm for the DPM models based on the CRP. Our algorithm is different from those of [Kurihara et al., 2009] and [Sato et al., 2009] in three ways: (i) it can handle an unfixd number of classes in mixture models, (ii) it does not require heuristics such as a purity, and (iii) it uses parallel processing in QA. The proposed algorithm (Eq. (4)) is easy to implement because it is similar to a classical CRP (Eq. (2)). That is, it is easy to apply the proposed algorithm to
other nonparametric models with which it is not easy to apply beam search, such as an infinite relational model \citep{Kemp2006}. The proposed algorithm will therefore be a promising new optimization technique when it is used with rapidly advancing multi core processors. As shown in Eq.\(2\), our algorithm is regarded as an optimization with a regularized term and its performance depends on parameter \(f\) like that other optimization algorithms with a regularized term does (e.g., L1 and L2 regularized optimization algorithms often used in machine learning). For future work, it will be worth analyzing what kind of schedule of \(f\) enables QA to work well.

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Appendix A. Proof of Theorem 3.1

We use the following Trotter product formula \citep{Trotter1959} to approximate

\[
p_{\text{QA}}(\sigma; \beta, \Gamma) = \frac{1}{Z} \sigma^\top e^{-\beta(H_e+H_o)} \sigma. \tag{A.1}
\]

If \(A_1, \ldots, A_L\) are symmetric matrices, we have

\[
\exp \left( \sum_{l=1}^L A_l \right) = \left[ \prod_{l=1}^L \exp(A_l/m) \right]^m + O \left( \frac{1}{m} \right). \tag{A.2}
\]

Applying the Trotter product formula to Eq.\(A.1\) with finite \(m\), we have

\[
p_{\text{QA}}(\sigma; \beta, \Gamma) = \frac{1}{Z} \sigma^\top e^{-\beta(H_e+H_o)} \sigma
\approx \frac{1}{Z} \sigma^\top \left( e^{-\frac{\beta}{m}H_e} e^{-\frac{\beta}{m}H_o} \right)^m \sigma. \tag{A.3}
\]

We evaluate the residual of this approximation. Since \(e^{A_1+A_2} = e^{A_1}e^{A_2}\) does not hold in general\(^4\) we need to use the Trotter product formula for computation. We rewrite \(\sigma\) as \(\sigma_1\) and note that

\[
\sigma_1^\top \left( e^{-\frac{\beta}{m}H_e} e^{-\frac{\beta}{m}H_o} \right)^m \sigma_1
= \sum_{\sigma_1} \ldots \sum_{\sigma_m} \sigma_1^\top e^{-\frac{\beta}{m}H_e} \sigma_1' \sigma_1^\top e^{-\frac{\beta}{m}H_o} \sigma_2
\ldots \sigma_m^\top e^{-\frac{\beta}{m}H_e} \sigma_m' \sigma_m^\top e^{-\frac{\beta}{m}H_o} \sigma_m+1
= \sum_{\sigma_1} \ldots \sum_{\sigma_m} \sum_{j=1}^m \sigma_j^\top e^{-\frac{\beta}{m}H_e} \sigma_j' \sigma_j^\top e^{-\frac{\beta}{m}H_o} \sigma_{j+1}, \tag{A.4}
\]

where \(\sigma_{m+1} = \sigma_1\). To express Eq.\(A.4\) more particularly, we use the following Lemma \text{Appendix A.1} and Lemma \text{Appendix A.2}.

Lemma Appendix A.1.

\[
\sigma_j^\top e^{-\frac{\beta}{m}H_e} \sigma_j' = \exp \left( -\frac{\beta}{m}E(\sigma_j) \right) \delta(\sigma_j, \sigma_j'), \tag{A.5}
\]

where \(\delta(\sigma_j, \sigma_j') = 1\) if \(\sigma_j = \sigma_j'\) and \(\delta(\sigma_j, \sigma_j') = 0\) otherwise.

Proof. By the definition, \(e^{-\frac{\beta}{m}H_e}\) is diagonal with \(e^{-\frac{\beta}{m}H_e}_{i,i} = E(\sigma_i)\), and \(\sigma_j\) and \(\sigma_j'\) are binary indicator vectors, i.e. only one element in \(\sigma_j\) is one and the others are zero. Thus, the above lemma holds.

Lemma Appendix A.2.

\[
\sigma_j^\top e^{-\frac{\beta}{m}H_o} \sigma_{j+1} = \left[ \sinh \left( \frac{\beta}{m} \Gamma \right) \right]^{2N}
\exp \left[ \sum_{i=1}^N \sum_{i=1}^N \delta(\tilde{\sigma}_j, i, i, n) \log \coth \left( \frac{\beta}{m} \Gamma \right) \right]. \tag{A.6}
\]

Proof. Using \((A \otimes B)(C \otimes D) = (AC) \otimes (BD)\) and

\(^4\)If \(A_1A_2 = A_2A_1\), then \(e^{A_1+A_2} = e^{A_1}e^{A_2}\).
Note that $\sigma$ and from Eq. (A.3), we have shown,

$$e^{\sigma_j^T e^{-\frac{1}{m} H_s \sigma_j + 1}} = e^{\sigma_j^T e^{-\frac{1}{m} l - \frac{l}{m} \sum_{i=1}^{N} \sum_{i=1}^{N} \sigma_{i,j}^T \sigma_{i,j}} + 1}$$

Using Lemma Appendix A.1 and Lemma Appendix A.2 into Eq. (A.7), we have

$$e^{\sum_{l=1}^{N} e^\sigma_j^T} = \prod_{i=1}^{N} \prod_{n=1}^{N} \prod_{j,i,n} \sigma_{j,i,n}^T \sigma_{j,i,n}.$$  \hspace{1cm} (A.7)

Note that $\sigma_j = \prod_{i=1}^{N} \prod_{n=1}^{N} \bar{\sigma}_{j,i,n}.$

$$e^{\sigma_j^T e^{-\frac{1}{m} H_s \sigma_j + 1}} = \left[1 + \frac{1}{2!} \left(\frac{\beta}{m} \Gamma\right)^2 + \cdots \right] E$$

$$+ \left[\frac{\beta}{m} \Gamma + \frac{1}{3!} \left(\frac{\beta}{m} \Gamma\right)^3 + \cdots \right] \sigma^\sigma$$

$$= \cosh \left(\frac{\beta}{m} \Gamma\right) E + \sinh \left(\frac{\beta}{m} \Gamma\right) \sigma^\sigma.$$ \hspace{1cm} (A.8)

Substituting Eq. (A.8) into Eq. (A.7), we have Eq. (A.9) because

$$\sigma_j^T \left[\cosh \left(\frac{\beta}{m} \Gamma\right) E + \sinh \left(\frac{\beta}{m} \Gamma\right) \sigma^\sigma\right] \bar{\sigma}_{j,i,n}$$

$$= \cosh \left(\frac{\beta}{m} \Gamma\right) \delta(\bar{\sigma}_{j,i,n} \bar{\sigma}_{j+1,i,n})$$

$$+ \sinh \left(\frac{\beta}{m} \Gamma\right) \left(1 - \delta(\bar{\sigma}_{j,i,n} \bar{\sigma}_{j+1,i,n})\right)$$ \hspace{1cm} (A.9)

Using Lemma Appendix A.1 and Lemma Appendix A.2 into Eq. (A.4),

$$\sigma_1^T \left(e^{-\frac{\theta}{m} H_s} e^{-\frac{\theta}{m} H_s}\right)^m \sigma_1$$

$$= \sum_{\sigma_2} \cdots \sum_{\sigma_m = 1}^{m} \exp \left[ -\frac{\beta}{m} E(\sigma) \right] \left[ \sinh \left(\frac{\beta}{m} \Gamma\right) \right]^{2N}$$

$$\exp \left[\sum_{i=1}^{N} \sum_{n=1}^{N} \delta(\bar{\sigma}_{j,i,n} \bar{\sigma}_{j+1,i,n}) \log \cosh \left(\frac{\beta}{m} \Gamma\right) \right].$$ \hspace{1cm} (A.10)

and from Eq. (A.3), we have shown,

$$p_{QA}(\sigma_1; \beta, \Gamma) \approx \sum_{\sigma_2} \cdots \sum_{\sigma_m} p_{QA-ST}(\sigma_1, \sigma_2, \ldots, \sigma_m; \beta, \Gamma).$$ \hspace{1cm} (A.11)

The same relation holds for $\sigma_2, \sigma_3, \ldots, \sigma_m.$

Appendix B. Derivation of Eq. (4)

Since

$$p_{QA}(\bar{\sigma}_{j,i}; \beta, \Gamma) \propto e^{-\frac{1}{m} E(\sigma_j) + (\beta, \Gamma) (\bar{\sigma}_{j,i} + \bar{\sigma}_{j,i} \sum_{i=1}^{N} \sum_{i=1}^{N} \bar{\sigma}_{i,j} \bar{\sigma}_{i,j})},$$

we have

$$p_{QA}(\bar{\sigma}_{j,i}; \beta, \Gamma) \propto \left(\frac{\sum_{i=1}^{N} e^{(\beta, \Gamma) (\bar{\sigma}_{j,i} + \bar{\sigma}_{j+1,i,n})}}{\alpha \sum_{i=1}^{N} \sum_{i=1}^{N} \bar{\sigma}_{j,i} \bar{\sigma}_{j+1,i,n}}\right)^{\frac{\beta}{N - 1 + \alpha}},$$

if $\bar{\sigma}_{j,i} \in \bar{\Sigma}_{j,i}, \{\rho_{j,i}^{(i)}\},$

if $\bar{\sigma}_{j,i} = \rho_{j,i}^{(i)}$,

if $\bar{\sigma}_{j,i} \notin \bar{\Sigma}_{j,i}.$ \hspace{1cm} (B.2)

This is easy to understand when you consider the meaning of $\bar{\delta}(\bar{\sigma}_{j-1,i}, \bar{\sigma}_{j,i}, \bar{\sigma}_{j+1,i})$ in multiple CRPs. $\bar{\delta}(\bar{\sigma}_{j-1,i}, \bar{\sigma}_{j,i}, \bar{\sigma}_{j+1,i})$ indicates the number of customers who share tables with the $i$-th customer in the $j$-1th and $j$+1th CRPs. Therefore, Eq. (4) is derived as another formulation of Eq. (B.2). Note that Eq. (4) is the approximation of Eq. (B.3).

Appendix C. Details of Network Model

In this section, we explain the Newman network model. $V$ is the vertex set. $v$ is a vertex; i.e., $v \in V$. $V$ is the number of vertices. $K$ is the number of classes. Suppose that the vertices fall into $K$ classes with probability $\pi_k$, where $\pi_k$ is the probability that a vertex is assigned to class $k$. Vertex $i$ belongs to class $k$, indicated by $z_i = k$. Each class has a probability $\phi_k$, which a link from a particular vertex in class $k$ connects to vertex $v$. A link from vertex $i$ to vertex $v$ is indicated by $\ell_i = v$. Each vertex links to other vertices in accordance
with \( \phi \). That is, vertex \( i \) links to vertex \( v \) in accordance with \( \phi_{z_i,v} \). The generation process for link \( \ell_i \) is represented by \( \ell_i \sim \text{Multi}(\phi_{z_i}) \), \( z_i \sim \text{Multi}(\tau) \), where \( \phi_{z_i} = (\phi_{z_1,1}, \phi_{z_2,2}, \ldots, \phi_{z_i,V}) \), and \( \text{Multi}(\cdot) \) is a multinomial distribution.

Suppose that \( \phi_k \) is distributed in accordance with the Dirichlet distribution \( H(\tau) \); i.e., \( \phi_k \sim H(\tau) \), where \( \tau \) is a parameter of the Dirichlet distribution. \( G \) is a random probability measure over \( \phi \); \( G \sim \text{DP}(\alpha, H(\tau)) \), where \( \text{DP}(\cdot) \) indicates the Dirichlet process (DP), \( \alpha \) is the DP concentration parameter that is equal to the hyper parameter of the CRP, and \( H \) is the base measure, which is the Dirichlet distribution here. The generation process for link \( \ell_i \) is represented by \( \ell_i \sim \text{Multi}(\phi_{z_i}), \phi_{z_i} \sim G \).

Here, we define \( A \) as an adjacency matrix with elements \( A_{iv} = 1 \) if there is an edge from \( i \) to \( v \); otherwise \( A_{iv} = 0 \). The probability of \( z_i \) given \( z_{\cdot i} = \{z_i \setminus z_i \} \) and adjacency matrix \( A \) is

\[
p(z_i = k|A, z_{\cdot i}; \alpha) \propto \quad \text{p}(A_i|z_i = k, A_{\cdot i}, z_{\cdot i})p(z_i = k|z_{\cdot i}; \alpha), (C.1)
\]

where \( A_i = (A_{i1}, A_{i2}, \ldots, A_{iV}) \), and \( A_{\cdot i} = A_i^\dagger A_i \).

We can calculate the probability of Eq. (C.1) as follows.

\[
p(A_i|z_i = k, A_{\cdot i}, z_{\cdot i}) = \frac{g(V\tau + \sum_u A_{uv}z_u^k)\prod_v g(\tau + \sum_{u \neq j} A_{uv}z_u^k)}{g(V\tau + \sum_u A_{uv}z_u^k)}
\]

where \( g(\cdot) \) is the gamma function, and \( z_u^k \) indicates 1 if \( z_i = k \); otherwise, it indicates 0.

\[
p(z_i = k|z_{\cdot i}; \alpha) = \begin{cases} \frac{N_{k-i}}{V - 1 + \alpha} & \text{(if } k \text{ previously used.)} \\ \frac{V - 1}{V - 1 + \alpha} & \text{(if } k \text{ is new.)} \end{cases} (C.3)
\]

where \( N_{k-i} \) is the number of vertices except vertex \( i \) assigned to class \( k \); i.e., \( N_{k-i} = \sum_{v \neq i} z_v^k \). We can adapt a Gibbs sampler for estimating \( z_i \) by using Eq. (C.1).

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