A Comparison of MCMC Sampling for Probabilistic Logic Programming

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Abstract. Markov Chain Monte Carlo (MCMC) methods are a class of algorithms used to perform approximate inference in probabilistic models. When direct sampling from a probability distribution is difficult, MCMC algorithms provide accurate results by constructing a Markov chain that gradually approximates the desired distribution. In this paper we describe and compare the performances of two MCMC sampling algorithms, Gibbs sampling and Metropolis Hastings sampling, with rejection sampling for probabilistic logic programs. In particular, we analyse the relation between execution time and number of samples and how fast each algorithm converges.

Keywords: Approximate Inference, Markov Chain Monte Carlo, Probabilistic Logic Programming.

1 Introduction

Probabilistic Logic Programming (PLP) is a useful paradigm for encoding models characterized by complex relations heavily depending on probability [10,13]. One of the main challenges of PLP is to find the probability distribution of query random variables, a task called *inference*. Real world problems often require very complex models. In this case, exact inference, which tries to compute the probability values in an exact way, is not feasible. Approximate inference overcomes this issue providing approximate results whose accuracy increases as the simulation continues. Markov Chain Monte Carlo methods are a class of algorithms used to perform approximate inference, especially when direct sampling from the probability distribution is not practical. In this paper we propose the first Gibbs sampling algorithm for PLP and we analyse how MCMC algorithms, Metropolis Hastings sampling and Gibbs sampling in particular, behave in terms of execution time and accuracy of the computed probability.

The paper is structured as follows: in Section 2 we introduce Probabilistic Logic Programming. In Section 3 we offer an overview of Markov Chain Monte

Carlo (MCMC) techniques and we analyse Metropolis Hastings sampling and Gibbs sampling. Section 4 shows the results of our experiments and Section 5 concludes the paper.

2 Probabilistic Logic Programming

Several approaches have been proposed for combining logic programming and probability theory. Here we consider languages based on the distribution semantics proposed by Sato in [15]. All the languages based on this semantics presented so far differ only in the way they encode choices for clauses but they all have the same expressive power [13].

A probabilistic logic program without function symbols defines a probability distribution over normal logic programs called *instances* or *worlds*. Logic Programs with Annotated Disjunctions (LPADs) [16] are a PLP language based on the distribution semantics. In these types of programs, the possible choices are encoded using annotated disjunctive heads of clause. An annotated disjunctive clause has the form $h_1 : \Pi_1; \ldots ; h_m : \Pi_m :- b_1, \ldots , b_n$, where $h_1, \ldots , h_m$ are logical atoms, $b_1, \ldots , b_n$ are logical literals and $\Pi_1, \ldots , \Pi_m$ are real numbers in the interval $[0, 1]$ that sum to 1. $b_1, \ldots , b_n$ is called *body* while $h_1 : \Pi_1; \ldots ; h_m : \Pi_m$ is called *head*. In case of $\sum_{k=1}^{m} \Pi_m < 1$, the head of the annotated disjunctive clause implicitly contains an extra atom *null* that does not appear in the body of any clause and whose annotation is $1 - \sum_{k=1}^{m} \Pi_m$.

Each world is obtained by selecting one atom from the head of each grounding (i.e. substitution of variables with terms in all possible ways) of each annotated disjunctive clause.

Consider the following LPAD:

$$\begin{array}{l} mistake(X) : 0.6 :- drunk(X). \\ mistake(X) : 0.7 :- bad\_player(X). \\ drunk(iverson). \\ bad\_player(iverson). \end{array}$$

This program can be read as: if X is drunk, then X makes a mistake with probability 0.6 and nothing happens with probability $1 - 0.6 = 0.4$. If X is a bad player, then X makes a mistake with probability 0.7 and nothing happens with probability 0.3. The last two clauses state that *iverson* certainly is a bad player and is drunk.

The probability of a query in a probabilistic logic program without function symbol is computed by extending the probability distribution over normal logic programs defined by the probabilistic logic program, to a joint distribution of the query and the worlds. Then, the probability is obtained by summing out the worlds. When a program contains also function symbols, the previous definition must be extended. This is because its grounding is infinite. So, the number of atomic choices in a selection that defines a world is infinite as well as the number of words. For a detailed definition see [12].

Performing inference, i.e. computing the probability distribution of the truth values of a query, can be done using exact or approximate methods. Exact inference can be performed in a reasonable time only when the size of the domain is relatively small, due to the #P-completeness of the task [7]. For larger domains, approximate inference is needed. Moreover, in programs with function symbols, goals may have an infinite number of possible infinite explanations and exact inference may not terminate [13]. Consider a one-dimensional random walk problem where a particle starts at position $X > 0$. At each time step, the particle can move one unit left (-1) or right $(+1)$ with equal probability. The walk stops as soon as the particle reaches 0. In this case, the walk terminates with probability one [5] but there is an infinite number of walks with nonzero probability [6]. In this example, exact inference, which tries to find the set of all explanations and then computing the probability of the query from it, will loop because the number of explanations is infinite.

Approximate algorithms using sampling are implemented in *cplint* [14] in the MCINTYRE [11] module. To be able to sample a query from a program, MCINTYRE applies a program transformation to the original program and then queries the modified program. Consider a disjunctive clause

$$C_i = h_{i1} : \Pi_{i1} \vee \ldots \vee h_{im_i} : \Pi_{im_i} :- b_{i1}, \ldots, b_{in_i},$$

where $\sum_{k=1}^{m_i} \Pi_{ik} = 1$. C_i is transformed into the set of clauses $MC(C_i) = \{MC(C_i, 1), \ldots, MC(C_i, m_i)\}$:

$$\begin{array}{ll} MC(C_i,1) = & h_{i1} :- b_{i1}, \ldots, b_{in_i}, \\ & \mathit{sample\_head}(PL, i, VC, NH), NH = 1. \\ \ldots & \\ MC(C_i,m_i) = & h_{im_i} :- b_{i1}, \ldots, b_{in_i}, \\ & \mathit{sample\_head}(PL, i, VC, NH), NH = m_i. \end{array}$$

where VC is a list containing each variable appearing in C_i and PL is a list containing $[\Pi_{i1}, \ldots, \Pi_{im_i}]$. If the parameters do not sum up to 1, the last clause (the one for *null*) is omitted. In other words, a new clause is constructed for each head. Then, using the predicate `sample_head/4`, a head index is sampled at the end of the body. If this index coincides with the head index, the derivation succeeds, otherwise it fails. The internal database of the SWI-Prolog engine [17] is used to record all samples (sampled random choices) taken with `sample_head/4` using the predicate `assertz/1`. Notice that `sample_head/4` is placed at the end of the body because at that point all the variables of the clause are ground (since we assume that the program is range restricted). The truth of a query in a sampled program can be tested by asking the query to the resulting normal program. This is equivalent to taking a sample of the query.

In general we are interested in computing approximate conditional probabilities: we want to compute the probability of an event $Y = y$ given that an event $E = e$ has been observed (i.e. $P(y \mid e)$) where Y and E are conjunctions of ground atoms and y and e are either true or false. In the rest of the paper we analyze three different algorithms available in *cplint* [14] for performing approximate inference with sampling: Gibbs sampling (Subsec. 3.1), Metropolis-Hastings (Subsec. 3.2) and rejection sampling.

Rejection sampling [7] is one of the simplest Monte Carlo algorithms. To take a sample of the query, it works in two steps: 1) it queries the evidence e. 2) If the query is successful, it queries the goal g in the same sample (that is, computing $P(g \mid e)$). Otherwise it discards the sample. The pseudocode for rejection sampling is shown in Algorithm 1.

Algorithm 1 Function Rejection: Rejection sampling algorithm.

```
1: function REJECTION SAMPLING($\mathcal{P}, query, evidence, Samples$)
2:     Input: Program $\mathcal{P}$, query, evidence, number of samples $Samples$
3:     Output: $P(query|evidence)$
4:     $Succ \leftarrow 0$
5:     $n \leftarrow 1$
6:     while $n \leq Samples$ do
7:         Call $evidence$
8:         if $evidence$ succeeds then
9:             Call $query$
10:            if $query$ succeeds then
11:                $Succ \leftarrow Succ + 1$
12:            end if
13:            $n \leftarrow n + 1$
14:        end if
15:    end while
16:    return $Succ/Samples$
17: end function
```

However, rejection sampling has a disadvantage: if the evidence is very unlikely, many samples are discarded, making the algorithm very slow. For example, if the probability of the evidence ($P(e)$) is very low, say 10^{-4}, then even for $N = 10^5$ samples the expected number of unrejected samples is 10. So, to obtain at least $Samples$ unrejected samples, we need to generate on average $N = Samples/P(e)$ samples from the distribution [7]. There are several alternatives to deal with low probability evidence, such as *likelihood weighting* [3] or Markov Chain Monte Carlo (MCMC) methods.

3 MCMC Sampling

Markov Chain Monte Carlo (MCMC) methods generate samples from the posterior distribution when directly sampling from the posterior is not feasible, due to the complexity of the distribution itself. The main idea of MCMC methods is to iteratively construct a Markov chain in which sampling can be done directly. As the number of samples increases, the approximation gets closer to the desired posterior distribution. In this way, MCMC methods are theoretically capable of getting arbitrarily close to the true posterior distribution. During the execution of MCMC algorithms, usually the first few samples are discarded because they may not represent the desired distribution. This phase is called *burnin* phase.

In this section we analyse two of the most famous MCMC sampling algorithms: Gibbs sampling and Metropolis Hastings sampling.

Algorithm 2 Function Gibbs: Gibbs MCMC algorithm

```
1: function Gibbs($query, evidence, Mixing, Samples, block$)
2:     GibbsCycle($query, evidence, Mixing, block$)
3:     return GibbsCycle($query, evidence, Samples, block$)
4: end function
5: function GibbsCycle($query, evidence, Samples, block$)
6:     $Succ \leftarrow 0$
7:     for $n \leftarrow 1 \rightarrow Samples$ do
8:         Save a copy of samples $C$
9:         SampleCycle($evidence$)
10:        Delete the copy of samples $C$
11:        $ListOfRemovedSamples$ = RemoveSamples($block$)
12:        Call $query$                ▷ new samples are asserted at the bottom of the list
13:        if $query$ succeeds then
14:            $Succ \leftarrow Succ + 1$
15:        end if
16:        CheckSamples($ListOfRemovedSamples$)
17:    end for
18:    return $\frac{Succ}{Samples}$
19: end function
20: procedure SampleCycle($evidence$)
21:    while $true$ do
22:        Call $evidence$
23:        if $evidence$ succeeds then
24:            $TrueEv \leftarrow true$
25:            return
26:        end if
27:        Erase all samples
28:        Restore samples copy $C$
29:    end while
30: end procedure
31: function RemoveSamples($block$)
32:    $SampleList \leftarrow []$
33:    for $b \leftarrow 1 \rightarrow block$ do
34:        retract sample $S = (Rule, Substitution, Value)$ ▷ samples are retracted from the top of
   the list
35:        Add $(Rule, Substitution)$ to $SampleList$
36:    end for
37:    return $SampleList$
38: end function
39: procedure CheckSamples($ListOfRemovedSamples$)
40:    for all $(Rule, Substitution) \in ListOfRemovedSamples$ do
41:        if $(Rule, Substitution)$ was not sampled then
42:            Sample a value for $(Rule, Substitution)$ and record it with assert
43:        end if
44:    end for
45: end procedure
```

3.1 Gibbs Sampling

The idea behind Gibbs sampling is the following: when sampling from a joint distribution is not feasible, we can sample each variable independently considering the other variables as observed [4]. In details, suppose we have n variables $X_1, \ldots, X_n$. First we set these variables to an initial value $x_1^{(0)}, \ldots, x_n^{(0)}$, for instance by sampling from a prior distribution. At each iteration (or until convergence) we take a sample $x_m^{(t)} \sim P(x_m \mid x_1^{t-1}, x_2^{t-1}, \ldots, x_{m-1}^{t-1}, x_{m+1}^{t-1}, \ldots, x_n^{t-1})$. There is also the possibility to perform blocked Gibbs sampling, i.e, group together two or more variables and sampling from their joint distribution conditioned on all other variables, instead of sampling each one individually.

Gibbs sampling is available on *cplint*. The code is shown in Algorithm 2. A list of sampled random choices is stored in memory using Prolog asserts. Function GibbsCycle performs the main loop. To take a sample, we query the evidence using function SampleCycle that performs a type of rejection sampling: it queries the evidence until the value true is obtained. When the evidence succeeds, we remove *block* random choices from the list of saved random choices using function RemoveSamples. Then, we ask the query and, if the query is successful, the number of successes is incremented by 1. The last step consist in calling function CheckSamples. This function checks if there are some rules not sampled in the list of removed random choices. If so, a value is sampled and stored in memory. This is due to the necessity of assigning a value to x_m even if it was not involved in the new derivation of the query. The probability is returned as the ratio between the number of successes and the total number of samples.

3.2 Metropolis Hastings

In Metropolis Hastings sampling, a Markov chain is built by taking an initial sample and, starting from this sample, by generating successors samples. Here we consider the algorithm developed in [9] and implemented in cplint [14]. Algorithm 3 goes as follows: 1) it samples random choices so that the evidence is true to build an initial sample. 2) It removes a fixed number (defined as *lag*) of sampled probabilistic choices to build the successor sample. 3) It queries again the evidence by sampling starting from the undeleted samples. 4) If the evidence succeeds, the query is asked by sampling. It is accepted with probability $min\{1, N_0/N_1\}$ where N_0 is the number of choices sampled in the previous sample and N_1 is the number of choices sampled in the current sample. 5) If the query succeeds in the last accepted sample then the number of successes of the query is increased by 1. 6) The final probability is computed as the number of successes over the total number of samples.

In details, function MH returns the probability of the query given the evidence. Function resample(lag) deletes *lag* choices from the sampled random choices. In [9] *lag* is always 1. Function InitialSample builds the initial sample with a meta-interpreter that starts with the goal and randomizes the order in which clauses are used for resolution during the search to make the initial sample unbiased. This is achieved by collecting all the clauses that match a subgoal and trying them in random order. Then the goal is queried using regular sampling.

4 Experiments

We tested the performances of Gibbs sampling, Metropolis Hastings sampling, and rejection sampling using four different programs. For each program, we ran the queries `mc_gibbs_sample/5`, `mc_mh_sample/5` and `mc_rejection_sample/5`

Algorithm 3 Function MH: Metropolis-Hastings MCMC algorithm

```
function MH($query, evidence, lag, Samples$)
    MHCycle($query, evidence, lag$)
    return MHCycle($query, evidence, Samples$)
end function
function MHCycle($query, evidence, Samples$)
    $TrueSamples \leftarrow 0$
    $Ssample \leftarrow$ InitialSample($evidence$)
    Call $query$
    if $query$ succeeds then
        $querySample \leftarrow true$
    else
        $querySample \leftarrow false$
    end if
    Save a copy of the current samples $C$
    $n \leftarrow 0$
    while $n < Samples$ do
        $n \leftarrow n + 1$
        $SamplesList \leftarrow$ Resample($lag$)
        Call $evidence$
        if $evidence$ succeeds then
            Call $query$
            if $query$ succeeds then
                $querySample' \leftarrow true$
            else
                $querySample' \leftarrow false$
            end if
            let $CurrentSampled$ be the current number of choices sampled
            if $min(1, \frac{CurrentSampled}{PreviousSampled}) > RandomValue(0, 1)$ then
                $PreviousSampled \leftarrow CurrentSampled$
                Delete the copy of the previous samples $C$
                Save a copy of the current samples $C$
                $querySample \leftarrow querySample'$
            else
                Erase all samples
                Restore samples copy $C$
            end if
        else
            Erase all samples
            Restore samples copy $C$
        end if
    end while
    Erase all samples
    Delete the copy of the previous samples $C$
    return $\frac{TrueSamples}{Samples}$
end function
function Resample($lag$)
    for $n \leftarrow 1 \rightarrow lag$ do
        Delete a sample $Sample$
        $NewSample \leftarrow$ Sample($Ssample$)
        Assert $NewSample$
    end for
    return $SamplesList$
end function
```

provided by the MCINTYRE module [11] implemented in cplint. All the algorithms are written in Prolog and tested in SWI-Prolog [17] version 8.1.7. For each query we show how the number of samples affects the execution time and the computed probability. All the experiments were conducted on a cluster[3] with Intel® Xeon® E5-2630v3 running at 2.40 GHz. Execution times are com-

[3] http://www.fe.infn.it/coka/doku.php?id=start

puted using the SWI-Prolog built-in predicate `statistics/2` with the keyword `walltime`. The results are averages of 10 runs. For both Gibbs and Metropolis Hastings sampling, we set the number of deleted samples (*burnin*) to 100.

For the first comparison, we consider a program that generatively defines a random arithmetic function[4]. The problem is to predict the value returned by the function given one or two couples of input-output, i.e., to compute a conditional probability. The peculiarity of this program is that it has an infinite number of explanations. As described in Section 2, approximate inference is needed, as exact inference may loop. In this example, the evidence has probability 0.05. Results are shown in Fig. 1. In this case, Metropolis Hastings sampling and Gibbs sampling have comparable execution time, but Gibbs sampling converges more slowly.

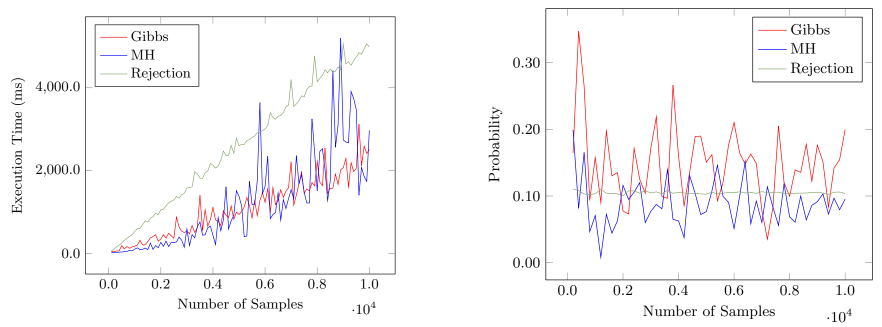


Fig. 1. Results for random arithmetic functions test.

The second program encodes a hidden Markov model (HMM) for modeling DNA sequences. The model has three states, `q1`, `q2` and `end`, and four output symbols, `a`, `c`, `g`, and `t`, corresponding to the four nucleotides (letters)[5] [2]. We compute the probability that the model emits the sequence `[a,c]` observing that from state `q1` the models emits the letter `a`. The evidence has probability 0.25. Results are shown in Fig. 2. In this case, all the three algorithms converge to the same probability value, but Metropolis Hastings is the slowest one with execution time several times larger than Gibbs and rejection sampling.

For the third test we consider a Latent Dirichlet Allocation (LDA) model[6] [1]. LDA is a generative probabilistic model especially useful in text analysis. In particular, it models the distribution of terms and topics in documents in order to predict the topic of the analysed text. This program, differently from the others, is hybrid, i.e., it contains also continuous random variables. For this

[4] http://cplint.eu/example/inference/arithm.pl
[5] http://cplint.eu/example/inference/hmm.pl
[6] http://cplint.eu/example/inference/lda.swinb

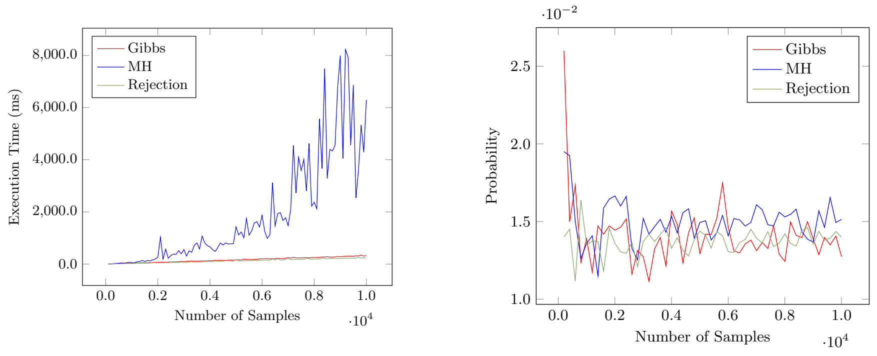
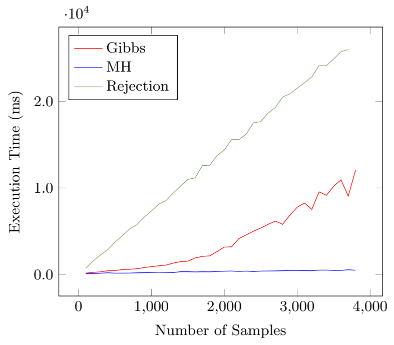


Fig. 2. Results for HMM test.

test, we fix both the number of words considered in a document (10) and the number of topics (2) and we compute the relation between number of samples, probability and execution time. In this example, we observe that the first two words of the document are equal, which has probability 0.01. The results are shown in Fig.3: in this case Gibbs sampling is slower than Metropolis Hastings both in execution time and number of samples needed to compute an accurate probability. Then we also fix the number of topics to 2 and increase the number of consecutive equal words from 1 to 8. In this test, the evidence is progressively extended, i.e., we observe that n number of words (from 1 to 8) are equal. In this case Metropolis Hastings sampling outperforms the other algorithms (Fig. 4 left). For Gibbs sampling and rejection sampling, the number of words in the plot is at most 6 since, for a value bigger than that, each query requires more than one hour of computation.

The last program describes a university domain[7] [8] characterized by students, professors and courses. Each professor is related to a course and each student attends a course. We are interested in computing the probability that a professor teaches a course given that the same professor is advisor of some students of the same course. We fixed the number of students to 10, and both the number of professors and courses to 1. In this case the evidence has probability 0.09. Results are shown in Fig. 5. As for the previous experiment, we also incremented the number of students up to 20 and plot how execution time changes (Fig. 4 right). In both cases, Gibbs sampling is still the slowest algorithm, but the performances are not so different from Metropolis Hastings and rejection sampling.

[7] http://cplint.eu/example/inference/uwcse.pl



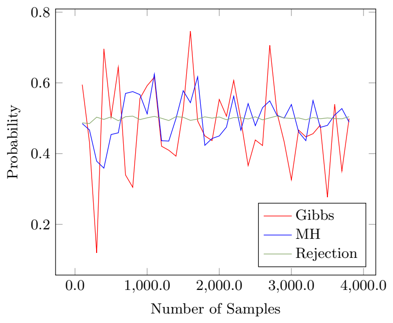
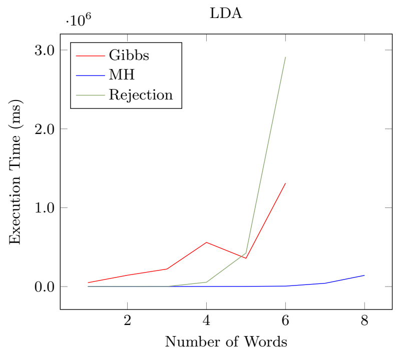


Fig. 3. Results for LDA model.



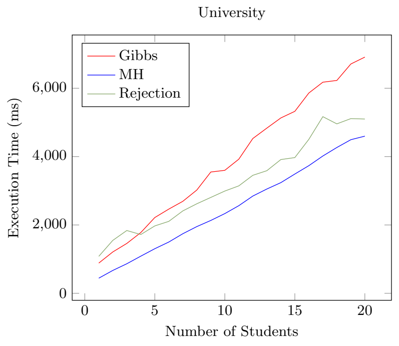


Fig. 4. Both graphs show how the number of facts affects the execution time. The left one is related to the LDA model while the right one to the university model. For both we fixed the number of samples to 10^4.

5 Conclusions

In this paper we proposed the first Gibbs sampling algorithm for PLP. We also compared it with Metropolis-Hastings and rejection sampling. The three algorithms are available in the cplint suite and online in the web application cplint.eu.

For each algorithm we conducted several experiments to compare execution time and convergence time. In three of the four experiments, Metropolis Hastings outperformed Gibbs sampling and rejection sampling in terms of accuracy and execution time. However, in the second experiment (HMM), Gibbs sampling has better performances than Metropolis Hastings and it is comparable to rejection sampling in terms of execution time. Also, in this test, Metropolis Hastings is the least accurate (it overestimates the probability) while Gibbs sampling and

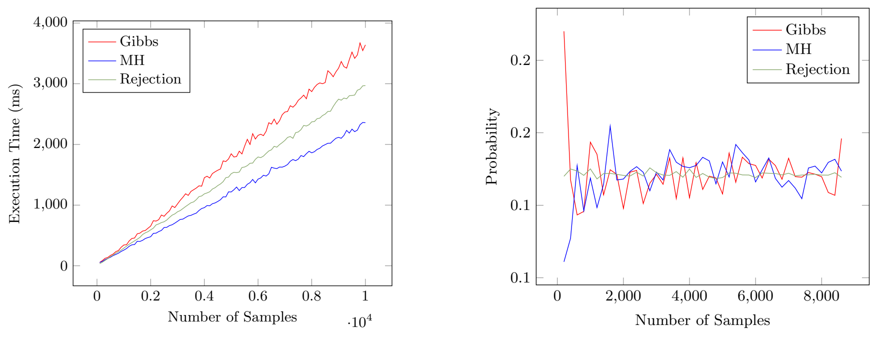


Fig. 5. Results for the university domain.

rejection sampling converge faster. Experimental analysis showed that Metropolis Hastings is the fastest among the three unless the evidence has a relatively high probability as in HMM where it has probability 0.25: in that case, Gibbs performs better.

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