Firefly Monte Carlo: Exact MC with data subsets

Feynman Liang, Max Chamberlin, Kai Xu

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1 Introduction

Many methods in Bayesian inference involve computing the likelihood $L(\theta)$ of parameters θ over iid observations $X = \{x_n\}_{n=1}^N$, defined as

$$L(\theta) = P(X|\theta) = \prod_{n=1}^{N} P(x_n|\theta) = \prod_{n=1}^{N} L_n(\theta)$$

For example, Monte Carlo Markov Chain (MCMC) are a class of methods often used to sample posterior distributions $P(\theta|X)$ with intractable partition functions $Z = \int P(X|\theta)P(\theta)d\theta$. When performing Metropolis-Hastings MCMC, at each iteration we need to compute the acceptance probability

$$A(\theta'|\theta) = \min\left\{1, \frac{q(\theta|\theta')L(\theta')P(\theta')}{q(\theta'|\theta)L(\theta)P(\theta)}\right\}$$

This means that each iteration requires at least one evaluation $L(\theta')$ of the likelihood over all N points ($L(\theta)$ can be cached from the prior iteration). Unfortunately, in the era of "Big Data" N may be on the order of petabytes and computing $L(\theta)$ at each iteration may be prohibitively expensive.

Rationale for selecting the paper:

We chose FlyMC because of the ubiquity of MCMC sampling methods which see use not just in the fields of machine learning and Bayesian statistics, but also in the fields of computational physics, biology and computational linguistics. If large speed-ups could be obtained using the methods expounded in FlyMC, this would be of great benefit to many different academic communities.

Furthermore, in Bayesian statistics, the recent development of MCMC methods has been a key step in making it possible to compute large hierarchical models that require integrations over hundreds or even thousands of unknown parameters, which is an exciting area of further research. However, to make MCMC work quickly for data of the order of that seen in the 'Big Data' era, any speed-up that is possible would be well received.

In addition to this, FlyMC is based on a mathematically elegant idea. The idea is that when performing inference, all that is necessary is to

2 Theory

The motivation for FlyMC is to achieve speed-ups over typical MCMC by estimating a large dataset's likelihood using smaller subsets of the data.

It also introduces auxiliary variables, which will act as indicators for the points for which the further computation (evaluations of $L_n(\theta)$) are required. This gives the motivation for the name, FlyMC, since these auxiliary variables can be thought of as lighting up when further likelihood evaluations are desired. Finally, with these terms in place, an intuitive explanation of FlyMc can be given. We have a lower bound for the likelihood, $B_n(\theta)$, which accounts for a large part of the probability mass on the distribution from θ. However, there is still a difference $L_n(\theta)$-$B_n(\theta)$, which we are uncertain of and which we would like to compute adjustments for through sampling. FlyMCn constructs a way of sampling from this residual probability mass, which is hopefully much smaller than $L_n(\theta)$, and so may result in large reductions in sampling time. The idea is neatly summarised in the graph below:

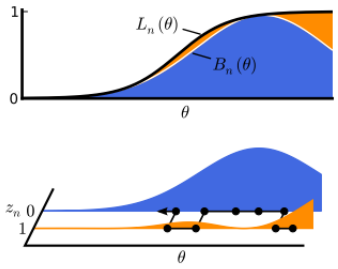


Figure 1: Graphical representation of the decomposition of L_n) into a $L_n - B_n$ part associated with bright variables $z_n = 0$ and a B_n part associated with dim variables $z_n = 0$ [MA14]

Firefly Monte Carly (FlyMC) is a method which addressses the computational problem of evaluating $L(\theta)$ for a large number of data points N through exact Monte Carlo estimates of the of the full dataset likelihood using smaller, tractable subsets. As an auxilliary variable method, it works by augmenting the joint distribution with hidden *brightness* variables$Z = \{z_n \in \{0,1\}\}_{n=1}^{N}$to form a *complete data likelihood*

$$P(X, Z|\theta) = \prod_{n=1}^{N} P(x_n|\theta)P(z_n|x_n, \theta)$$

Notice that we can recover the desired likelihoods simply through marginalization

$$\sum_{Z} P(X, Z|\theta) = \sum_{z_1} \cdots \sum_{z_N} \prod_{n=1}^{N} P(|x_n|\theta)P(z_n|x_n, \theta) = \prod_{n=1}^{N} P(|x_n|\theta) \sum_{z_n} P(z_n|x_n, \theta) = L(\theta)$$

In FlyMC, the brightness variables are chosen to have Bernoulli distribution

$$P(z_n|x_n, \theta) = \left(\frac{L_n(\theta) - B_n(\theta)}{L_n(\theta)}\right)^{z_n} \left(\frac{B_n(\theta)}{L_n(\theta)}\right)^{1-z_n} \tag{1}$$

where$B_n(\theta)$ is a lower bound on the likelihood satisfying

$$0 \leq B_n(\theta) \leq L_n(\theta) \tag{2}$$

$$\prod_{n \in A} B_n(\theta) \text{ can be efficiently computed for any data subset } A \subset X \tag{3}$$

2 is required for 1 to be a valid probability distribution. To see why 3 is necessary, consider computing the complete data likelihood

$$
\begin{aligned}
P(X, Z|\theta) &= \prod_{n=1}^{N} P(x_n|\theta)P(z_n|x_n, \theta) \\
&= \prod_{n=1}^{N} L_n(\theta) \left(\frac{L_n(\theta) - B_n(\theta)}{L_n(\theta)}\right)^{z_n} \left(\frac{B_n(\theta)}{L_n(\theta)}\right)^{1-z_n} \\
&= \prod_{x_n \in X_{bright}} (L_n(\theta) - B_n(\theta)) \prod_{x_n \in X_{dim}} (B_n(\theta)) \qquad (4) \\
&= \prod_{n=1}^{N} B_n(\theta) \prod_{x_n \in X_{bright}} \frac{L_n(\theta) - B_n(\theta)}{B_n(\theta)} \qquad (5)
\end{aligned}
$$

where the bright points $X_{bright} = \{x_n : z_n = 1\}$ and dim points $X_{dim} = \{x_n : z_n = 0\}$give rise to the "Firefly" in the paper title. Notice that as a consequence of our choice for1,4 decomposes into two products where $\frac{L_n(\theta)-B_n(\theta)}{B_n(\theta)}$ only needs to be evaluated for $x_n \in X_{bright}$. By assuming 3, the other term $\prod_{n=1}^{N} B_n(\theta)$ can be efficiently computed so the computational complexity is determined by X_{bright}.

2.1 Performance comparison

Instead of evaluating $L_n(\theta)$ over all N points, FlyMC only evaluates the likelihood over a subset of points X_{bright}. This provides a speedup of $\frac{N}{\#X_{bright}}$per iteration. However, since the brightness variables $z_n$are themselves, to understand the performance improvements we consider the expected number of bright points $E[\#X_{bright}]$.

Note that for any point x_n,1 implies the probability $x_n$is bright is given by $\frac{L_n(\theta)-B_n(\theta)}{L_n(\theta)}$. Hence, the number of bright points is given by

$$
E[\#X_{bright}] = \sum_{n=1}^{N} E[z_n] = \sum_{n=1}^{N} \int P(\theta|X) \frac{L_n(\theta) - B_n(\theta)}{L_n(\theta)} d\theta \qquad (6)
$$

This says that the number of bright points (and hence the speedup achieved by FlyMC) is related to the gap between the true likelihood $L_n(\theta)$ and the lower bound $B_n(\theta)$, weighted by the posterior $P(\theta|X)$.

This result makes intuitive sense. Consider the extreme case where for all n: $B_n(\theta) = 0$. Then $P(z_n = 1|x_n, \theta) = 1$ so every data point is bright (i.e. $X = X_{bright}$) and 4 reduces to evaluating the full dataset likelihood $\prod_{n=1}^{N} L_n(\theta)$ as usual.

In the other extreme, if $B_n(\theta) = L_n(\theta)$ so all data points are dim. At first it appears that FlyMC counterintuitively offers a $\frac{N}{\#X_{bright}} = \frac{N}{0} = \infty$speedup. However, considering 4 reveals that what is computed is $\prod_{n=1}^{N} B_n(\theta) = \prod_{n=1}^{N} L_n(\theta)$, which by assumption 3can be computed efficiently. But then computing $L(\theta) = \prod_{n=1}^{N} L_n(\theta)$ is efficient and hence is no longer $O(N)$, contradicting our earlier assumptions.

2.2 Discussion on the lower bound $B_n(\theta)$

The integral role played by the lower bound $B_n(\theta)$ makes it an important topic of investigation. In this section, we investigate how reasonable and justified are the assumptions required for developing FlyMC's theory.

One of our assumptions (3) was that computation of $\prod_{n=1}^{N} B_n(\theta)$ be efficient new θ. For example, choosing $B_n(\theta)$ to be exponential family will make computing $\prod_{n=1}^{N} B_n(\theta)$ for each new θ be $O(1)$ because

$$
\begin{aligned}
B_n(\theta) &\propto \exp(\langle \eta_n, T(\theta) \rangle) \\
\prod_{n=1}^{N} B_n(\theta) &\propto \exp(\langle \sum_{n=1}^{N} \eta_n, T(\theta) \rangle)
\end{aligned}
$$

and $\sum_{n=1}^{N} \eta_n$ can be evaluated once and cached. We believe that this assumption is quite restrictive and have had some difficulty coming up with functional forms which are not exponential family that satisfy this assumption.

The other assumption (2) required $B_n(\theta)$ be a non-negative lower bound for $L_n(\theta)$. This is trivially satisfied by setting $B_n(\theta) = 0$, but to be practical we should try to find a lower bound with the smallest gap possible. Several forms of bounds exist for commonly used likelihoods; the original authors consider the Jaakola and Jordan bound on the log logistic function. However, this requirement is quite restrictive and unrealistic for more complex use

cases. For example, if $L_n(\theta)$ is given by some complicated Bayes net or neural network, then a valid $B_n(\theta)$ for use with FlyMC is not immediately obvious.

2.2.1 MAP-tuning the lower bound

In certain cases (e.g. Jaakola and Jordan bound on log logistic), B_n is part of a parametric family of lower bounds $\{B_n(\cdot, \xi)\}_\xi$where ξ is a free parameter. Since the number of bright points determines the speedup offered by FlyMC, 6 suggests that we should choose ξ to minimize $E\left[\frac{L_n(\theta)-B_n(\theta)}{L_n(\theta)}\right]$ for each datapoint n where the expectation is taken over the posterior distribution $P(\theta|X)$.

The authors of FlyMC propose a *MAP-tuned FlyMC* variant where the posterior expectation $E\left[\frac{L_n(\theta)-B_n(\theta)}{L_n(\theta)}\right]$ is replaced with the MAP point estimate $\frac{L_n(\theta_{MAP})-B_n(\theta_{MAP})}{L_n(\theta_{MAP})}$ and$\xi = \text{argmin}_\xi L_n(\theta_{MAP}) - B_n(\theta_{MAP})$.$\theta_{MAP} = \text{argmax}_\theta P(\theta|X)$ can be found using stochastic gradient descent to handle large data-set concerns.

Our opinions about this method are mixed. While MAP tuning should provide a tighter lower bound than no tuning, approximating the posterior with a delta distribution centered at θ_{MAP}seems suspicious. Other methods which could be considered here include first generating some posterior samples using an untuned chain or MCMC on a subset of the data, then tuning ξover the posterior samples.

3 Implementation

FlyMC augments traditional MCMC by introducing brightness variables Z which are Gibbs sampled along with the original chain's state θ. At a high level, the algorithm consists of the following steps:

1. Initialize $\theta^{(0)}$
2. For $t = 1, \cdots, N_{iter}$
   (a) For $n = 1, \cdots, N$: sample $z_n^{(t)} \sim \text{Bernoulli}\left(\frac{L_n(\theta^{(t)})-B_n(\theta^{(t)})}{L_n(\theta^{(t)})}\right)$ with $\theta = \theta^{(t)}$fixed
3. Propose $\theta^{(t+1)} \sim q(\theta^{(t+1)}|\theta^{(t)})$
4. Compute acceptance probability $A(\theta^{(t+1)}|\theta^{(t)}) = \min\left\{1, \frac{q(\theta^{(t)}|\theta^{(t+1)})P(X,Z|\theta^{(t+1)})P(\theta^{(t+1)})}{q(\theta^{(t+1)}|\theta^{(t)})P(X,Z|\theta^{(t)})P(\theta^{(t)})}\right\}$
5. Repeat from step 2 until chain has mixed, yielding a single sample $z_n^{(\infty)}$

In step 4, the complete data likelihood is computed using 4 and hence only requires evaluating the likelihood over X_{bright}.

One possible criticism of the method described above is that step 2(a) requires sampling $z_n$from N Bernoulli distributions each with probability $\frac{L_n(\theta)-B_n(\theta)}{L_n(\theta)}$ and hence direct sampling will again require N evaluations of $L_n(\theta)$. Fortunately, this can be avoided through *implicit sampling*, where a second MH-MCMC is used to sample the z_i. The motivation is that ideally many $z_i = 0$ so it makes sense to only consider proposals where each dim point has a small $q_{d\to b} \in [0, 1]$ probability of becoming bright. Then, evaluating the acceptance probability only requires computing $L_n(\theta)$ at the $z_n$which have been proposed to change state.

3.1 Provided reference software

Reference code is provided by the authors[1], which provides implementations FlyMC for logistic regression using MH-MCMC, softmax using Langevin dynamics, and sparse linear regression using slice sampling. The reference implementation includes an implicit sampling scheme for sampling brightness variables z_i.

3.2 Our contributions to the project

However, the only full example provided is a logistic regression example on toy data and is insufficient for reproducing the results reported in the paper. We forked he authors' code [2] and added our own modifications, most importantly:

1. Support for MAP-tuning of the lower bounds, using scipy.optimize for MAP estimation
2. Implementation of regular full-dataset MCMC, which is achieved by fixing $\forall i : z_i = 1$

[1] https://github.com/HIPS/firefly-monte-carlo
[2] https://github.com/feynmanliang/firefly-monte-carlo

3. Improved numerical overflow handling in `LogisticModel`

4. Instrumentation for counting log-likelihood evaluations and outputting traces of chain state and log likelihood per iteration

5. Integration, parameter tuning, and reproduction of MNIST Logistic Regression, CIFAR-10 Softmax Classification, and Robust Linear Regression experimental results

We also fixed a significant bug in some caching code provided with the reference implementation and submitted our bugfix back upstream [3]. The problem was that computations of $\left\{\frac{L_n(\theta)-B_n(\theta)}{B_n(\theta)} : n \in idx\right\}$were being cached for vectors θ and idx, but that caching was performed over the entire idx vector rather than elementwise. For example, if $idx2 \subsetneq idx$, then even though $\left\{\frac{L_n(\theta)-B_n(\theta)}{B_n(\theta)} : n \in idx2\right\} \subset \left\{\frac{L_n(\theta)-B_n(\theta)}{B_n(\theta)} : n \in idx\right\}$ the reference implementation would still result in a cache miss because $idx2 \neq idx$. This bug causes the number of likelihood evaluations to be twice the number of proposed bright points $\#X_{bright}$at each iteration, which means that FlyMC will only offer speedups if $\#X_{bright} < \frac{N}{2}$.

4 Reproduction experiments

The Experiments to be replicated:

In this practical, we conducted the following three experiments:

- Logistic regression: For this particular task, we tested we tested FlyMC's preformance for the task of classifying 7s and 9s on MNIST, with prior $P(\theta) \sim \mathcal{N}(0, I)$.
- Softmax classification: For this task, we tested FlyMC's ability to fit a softmax classification model on three CIFAR-10 classes (airplane, automobile and bird) using Langevin dynamics
- Robust linear regression: For logistic regression task, we generated synthetic data and evaluated the performance of FlyMC in comparison to regular MCMC.

The first two of these three experiments were data-sets used in the paper. However, for the third data-set we decided it would be intersting to see if the same results claimed by a paper could be found in a data-set that was not hand-picked by the authors.

Results

The plots of autocorrelation from the three data-sets display the same general trends. The autocorrelation curve for MCMC is below that of FlyMC and FlyMap. These results tend to show that FlyMC variant tends to produce samples θ that have have a greater dependence between themselves. This is unsurprising given that there are fewer likelihood evaluations at each step of FlyMC, which means that there are fewer updates to the posterior of $p(\theta\ |\theta)$.

A further trend that can be noticed is that, at least initially, the negative log posterior for MCMC tends to be greater than either two of the FlyMC variants. This is unsurprising, because at any given iteration, MCMC , will have computed a great deal more likelihood updates for many more points, and so the posterior probabilities of the sampled parameter theta under MCMC, will have had more of an opportunity to adapt to the data-set given than the Fly variants (at any given iteration).

For both soft-max classification and logistic regression, the number of log-likelihood evaluations at each step remains constant. This is to be expected, since likelihood updates are computed for all the data-points. However, because the parameters for the regression data are sampled using slice-sampling (which essentially involves an adaptive step size) the number of likelihood evaluation tends to oscillate up and down depending on the weight of the step size.

That not withstanding, in all cases FLyMC computes likelihood evaluations that are an order of magnitude smaller than MCMC. For MNIST logistic regression, approximately 1/12 of the likelihoods are computed at each stage. For softmax classification, FlyMC evaluated roughly 1/3 of the likelihoods that regular MCMC evaluated and FlyMap performed even better evaluating only 1/6 of the likelihoods that regular MCMC evaluated at each step.

Without belabouring the point much further, we can see that exactly the right trends are being seen as we would expect for data of this sort: MCMC has better mixing, and better likelihoods for a given iteration; whereas FlyMC and FlyMap show worse mixing, and have lower negative log likelihoods at a given iteration, but crucially

[3] https://github.com/HIPS/firefly-monte-carlo/pull/1

use fewer log-likelihood updates at each iteration. These are exactly the same sorts of trends that are seen in the original paper. Having looked at the plots, the next key quantity that ought to be observed is the effective sample rate.

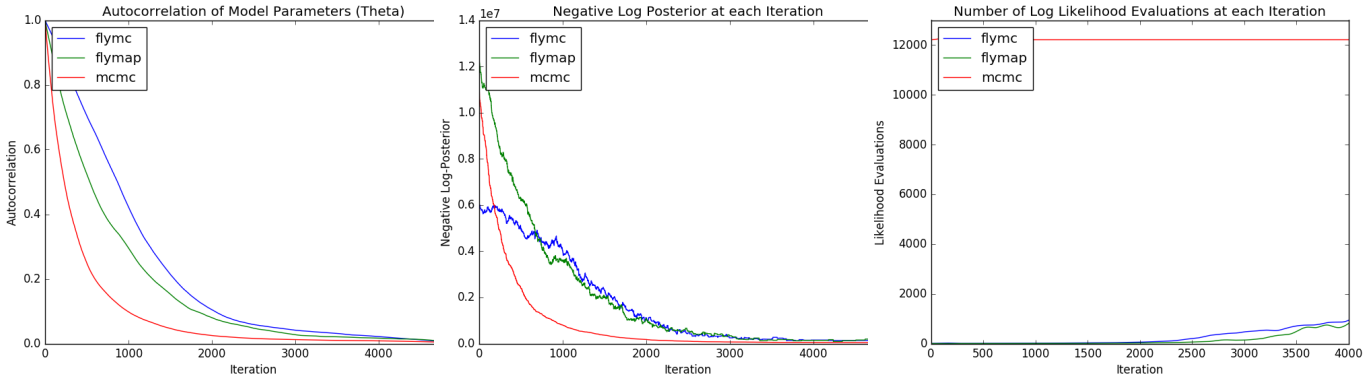
We can calculate a quantity that determines the effective sample rate by choosing a log-likelihod value, L, and computing the number of iterations MCMC, FlyMap and FlyMC took to reach that log likelihood. Suppose these numbers were M, FM and FMC respectively for each of MCMC, FlyMap and FlyMC. Then for FlyMap, the effective sample rate is given by: (FM/M)*average number of likelihood evaluations up until FM. I present our estimates of these evaluations in Table **??**Table 1. The results are based using, the corresponding MCMC sampler.

shows the effective sample size (ESS) of regular MCMC, untuned MCMC and MAP-tuned FlyMC for the three experiments.

Table 1: ESS of regular MCMC, untuned MCMC and MAP-tuned FlyMC for the three experiments

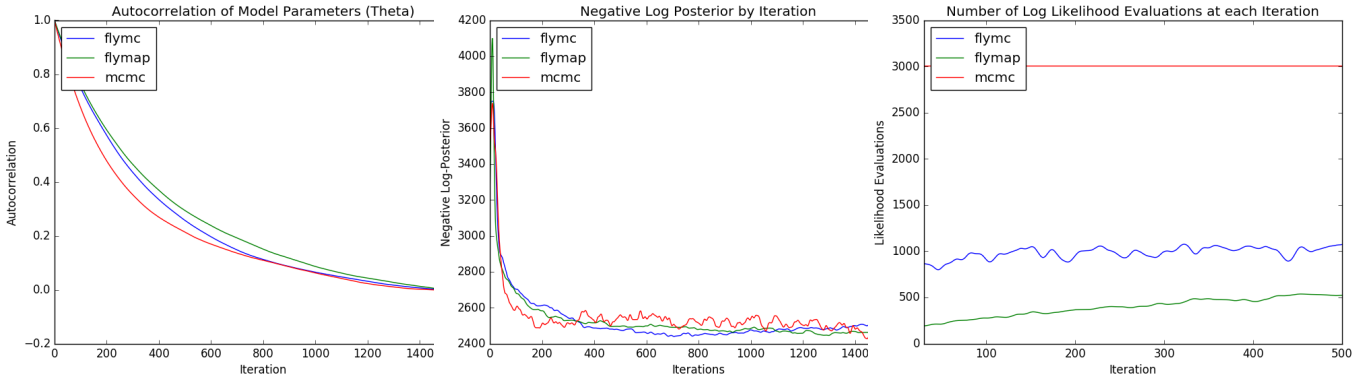
	Regular MCMC	Untuned FlyMC	MAP-tuned FlyMC
Logistic regression	3.6	0.5	0.6
Softmax clssification	7.1	4.0	3.3
Robust regression	1.1	1.0	1.1

With the SSE from the table and the speedup observed from the plots of number of log-likelihood evaluations per iteration, we can conclude that MAP-tuned FlyMC provides a reasonable speedup while the untuned one is slower than the regular one.



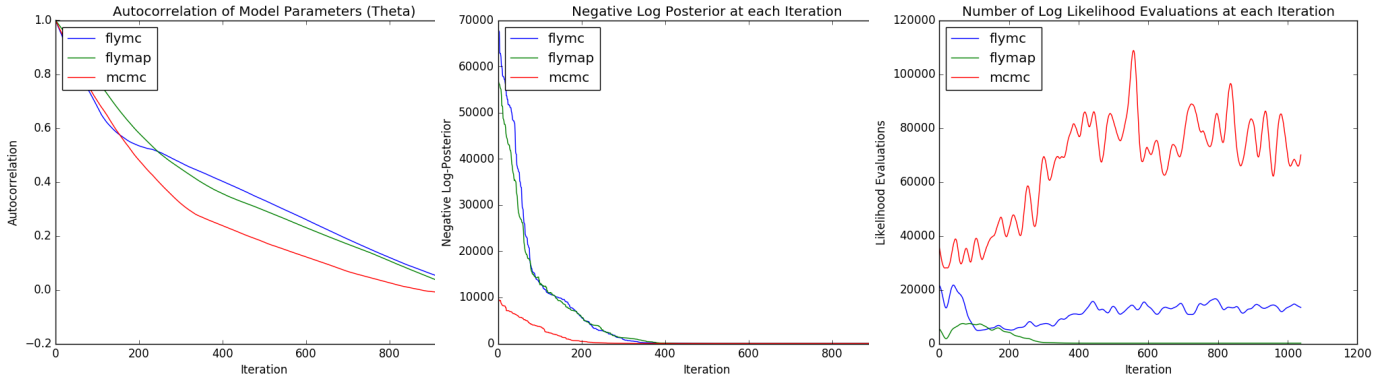
(a) Autocorrelation (b) Negative log posterior (c) Number likelihood evaluations

Figure 2: Logistic regression binary classification on MNIST with MH-MCMC



(a) Autocorrelation (b) Negative log posterior (c) Number likelihood evaluations

Figure 3: Softmax 3-way classification on CIFAR-10 with Langevin dynamics



(a) Autocorrelation (b) Negative log posterior (c) Number likelihood evaluations

Figure 4: Robust regression on synthesized data with slice sampler

5 Conclusion

You should end by critically evaluating your work and suggest what you would have done given more time.

From this practical, we learned that FlyMC is n elegant framework for MCMC sampling that can lead into speed-ups of an order of magnitude greater than what has been seen with conventional MCMC samplers. Map-tuning FlyMC, yielded the fastest samplers with effective sampling weights as low as 20 times that of traditional MCMC.

As a summary of the work undertaken, our practical implementation of Firefly MC led, which was based on the code provided by HIPs, led to several important pull requests on Github which fixed the caching of bright variables. in addition, we had to produce plots, tune parameters, and amend the sampling procedure so that they would work with the various kinds of data that was investigated in the paper.

A thorough grounding into the underpinning mathematical background of FlyMc was also given.

We replicated almost almost all the graphs and figures in the paper, however, we would have liked to generate more tabulated data on effective sample rates than we could have.

Many extensions of the work we have presented are possible. One particularly important experiment would be to tune the lower bounds over multiple parameter values sampled from the posterior rather than the single MAP estimate. This would ensure a low number of expected bright points, even if we are possibly far away from the MAP estimate. Given the significant performance difference tuning lower bounds in this manner to yield even lower numbers of bright points and hence greater speedups over traditional MCMC.

Another direction for investigation is on the lower bounds B_n. The assumptions made in assumptions 1 and 2 on B_n are required for formulating FlyMC, and the authors do a good first pass discussion about using exponential families for B_n. However, it may be interesting to consider other functional forms for B_n such that $\prod_{n=1}^{N} B_n(\theta)$ is cheap to compute. Furthermore, it is often the case that we are working with likelihoods $L(\theta)$ which do not have a well-known lower bound (e.g. $L(\theta)$ could be parameterized by a deep neural network). In these situations, one would like any form of lower bound which is non-zero. Alternatively, one could investigate what happens when approximate bounds are used for $B_n(\theta)$ where cite the 0 <= Bn <= 1 does not hold for all θ.

Finally, we would like to mention that although the motivation for this work is computing on big datasets with large N, most experiments presented here and in the paper were small and run on a single machine. For FlyMC to truly be impactful in big data applications, an implementation on a distributed computing platform (e.g. Spark, Hadoop) which demonstrates tractable MCMC on large datacenter-scale datasets would be a convincing and immediately useful line of work.

References

[MA14] Dougal Maclaurin and Ryan P Adams. Firefly monte carlo: Exact mcmc with subsets of data. *arXiv preprint arXiv:1403.5693*, 2014.