Comment: A brief survey of the current state of play for Bayesian computation in data science at big-data scale

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We wish to contribute to the discussion of this interesting paper by offering our views on the current best methods for Bayesian computation, both at Big-Data scale and with smaller data sets, as summarized in Table 1. This table is certainly an over-simplification of a highly complicated area of research in constant (present and likely future) flux, but we believe that constructing summaries of this type is worthwhile despite their drawbacks, if only to facilitate further discussion.

The entries in the table are tailored to problems—such as classification and regression—in which the data set is organized into $n$ rows (representing subjects of study, which may or may not be organized hierarchically, for example, patients nested in hospitals) and $p$ columns of variables measured on the subjects, but the table may be relevant for other data structures as well (for example, data sets in topic modeling (e.g., Blei, 2012) may be visualized as consisting of $n$ words (nested inside documents) and $p$ topics). The rows of Table 1 play out the four combinations of big and small $n$ and $p$, and the columns identify the four major hardware configurations currently available: single CPU, single GPU, cluster of CPUs, and cluster of GPUs. A more detailed table would have broken both $n$ and $p$ out into (small, medium, large), and further detail could have been supplied in a more model-specific fashion, but in our view Table 1 already makes some interesting comparisons.

For us, “Big Data” refers to settings in which the available data set is too big to store and process in memory on a single machine, or worker (consisting of one single-threaded CPU, some RAM, and some disk storage). In our table this corresponds to big $n$, which in today’s environment typically equates to a data set that takes tens of gigabytes (or more) to store. For our purposes, big $p$ is in the hundreds of thousands, tiny $p$ is a few hundred, and small $p$ is in between.

Our comments on the individual cells in the table are as follows.

- $(n, p) = (\text{Small, Small})$ is the current Bayesian computational comfort zone: an example would be logistic regression using a regularization prior (e.g., the horseshoe (Carvalho, Polson and Scott, 2010)) with an $n$ of a few thousand and $p$ on the order of 100.
Table 1  Our view of the current best methods for simulation-based Bayesian computation, as a function of number of observations (n), number of predictors (p), and available hardware. Big n specifies data sets that take tens of gigabytes (or more) to store; tiny p is a few hundred; big p is hundreds of thousands.

| n       | p       | Single CPU                        | Single GPU                        | CPU Cluster                  | GPU Cluster
|---------|---------|-----------------------------------|-----------------------------------|------------------------------|----------------
| Small   | Small   | Standard MCMC                     | GPU-accelerated particle filters  | Independent parallel chains  | not needed     |
| Small   | Big     | Hamiltonian Monte Carlo (HMC) or Gibbs sampling\(^{(1)}\) | HMC or GPU-accelerated Gibbs sampling | Asynchronous Gibbs sampling\(^{(2)}\) | No current Bayesian method |
| Big     | Small   | Continuous-time MCMC with subsampling and control variates\(^{(3)}\) | Continuous-time MCMC or GPU-accelerated Gibbs sampling\(^{(4)}\) | Asynchronous Gibbs sampling\(^{(5)}\) or methods based on sharding | No current Bayesian method |
| Big     | Big     | Hopeless: point estimates only     | Model-specific\(^{(6)}\)           | Model-specific\(^{(7)}\)     | No current Bayesian method |

\(^{(1)}\) HMC if gradient is available, else Gibbs.
\(^{(2)}\) The exact algorithm if Metropolis–Hastings correction is cheap enough, otherwise the approximate algorithm if diagnostic indicates appropriate.
\(^{(3)}\) If gradient is available and p is tiny.
\(^{(4)}\) ZigZag (see text) or BPS with parallel gradient evaluations if p is tiny; GPU-accelerated Gibbs if gradient unavailable and/or p is medium-size.
\(^{(5)}\) If data augmentation is possible with the model under study.
\(^{(6)}\) May be possible for gradient-based methods in some models (current research).
\(^{(7)}\) An example is topic modeling, using AD–LDA (approximate) or Pólya Urn LDA (essentially exact with big n).

– Standard MCMC on a single CPU is fine here, with home-grown code or using an environment such as WinBUGS (Lunn et al., 2000) or RJAGS (Plummer, 2003).

– If you have a single GPU and need answers extremely quickly, GPU-accelerated particle filters (Lee et al., 2010) are a good option with some models.

– If instead you have access to a cluster of workers, you can of course readily run independent parallel chains on each worker and merge the results. This includes computing on a single machine with multiple cores/threads, for example via doParallel or snow in R.

– A cluster of GPUs would be overkill in this situation.
- $(n, p) = (\text{Small, Big})$ is already at the research frontier with some hardware configurations.
  - Using a single worker, you can do Hamiltonian Monte Carlo (HMC, Betancourt, 2017) if the gradient of the log posterior is available (e.g., with non-discrete likelihoods), writing the code yourself or fitting your model in Stan (Stan Development Team, 2016), or you can use Gibbs sampling in settings with or without a gradient.
  - With a single GPU, HMC is again a good option with a gradient (Beam, Ghosh and Doyle, 2016), or you can use GPU-accelerated Gibbs sampling (Terenin, Dong and Draper, 2016). The latter method can be better in models with heavy-tailed error distributions, where HMC sometimes performs poorly, but HMC within Gibbs would be even better than pure Gibbs in such problems.
  - If you have access to a cluster of CPUs, one good method is asynchronous Gibbs sampling (Terenin, Simpson and Draper, 2017), using either (a) the exact algorithm, if the Metropolis-Hastings correction built into the method is cheap enough or (b) the (much faster) approximate algorithm, if the diagnostic described in the paper indicates that this is safe.
  - It would appear that no one knows how to make efficient fully Bayesian use of a GPU cluster at present: the problem is that GPU computation is massively faster than available network speed, so it’s typically not at all clear how to keep all of the GPUs busy at once.

- $(n, p) = (\text{Big, Small})$ is an active area of recent and current research.
  - On a single CPU, in our view the most promising approach with big $n$ and tiny $p$, when a gradient is available, involves methods based on creating continuous-time stochastic processes without discretization that sample correctly from the posterior of interest—these include ScaLE (Pollock et al., 2016), ZigZag sampling (Bierkens, Fearnhead and Roberts, 2016), and the Bouncy Particle Sampler (BPS, Bouchard-Côté, Vollmer and Doucet, 2015). The key advantage of these methods is the ability to run while evaluating one data point at a time.
  - With a single GPU, two good options are (a) BPS (with parallel gradient evaluations) if $p$ is tiny and (b) GPU-accelerated Gibbs sampling if the gradient is unavailable and/or if $p$ is medium in size (up to 10,000, say).
  - A cluster of workers at your disposal lands you in the cell into which Steve Scott’s present paper fits, under divide-and-conquer methods based on sharding—other methods that partition the data set into small subsets of subjects, make standard calculations on each small data set, and then combine at the end include a variety of techniques developed by David Dunson and his collaborators (e.g., Srivastava, Li and Dunson, 2015). Many of the sharding papers concentrate on examples in which $p$ is tiny;
Asynchronous Gibbs sampling is a good alternative with larger $p$ when data augmentation is possible in the model at hand. One of the issues that sharding-based methods face with larger $p$ is ensuring convergence on each of the individual shards.

- With a cluster of GPUs, as noted above, the profession is currently at a loss to make fully effective use of the hardware for posterior exploration (as opposed to optimization: see below).

* $(n, p) = (\text{Big, Big})$ is where current methods start to reveal their (serious) limitations.

- Using only a single CPU, fully Bayesian posterior exploration in this case is hopeless. The best you can hope for is employing optimization-based methods to obtain the maximum a posteriori (MAP) estimate. As a large body of work in machine learning shows, this is sometimes adequate to solve the problem at hand.

- With a single GPU, success becomes model-specific. It may be possible to adapt gradient-based methods to drive a GPU efficiently in some models—this is a topic of current research.

- Employing a cluster of workers, with $n$ and $p$ both big, good results are currently also available only on a model-specific basis—topic models provide an example, with Approximate Distributed LDA (AD–LDA, Newman et al., 2009) offering approximate results and Pólya Urn LDA (Terenin et al., 2017) producing answers that are exact up to Monte Carlo noise with big $n$. If it’s sufficient to obtain MAP estimates in the problem you’re working on, by far the best Big-Data optimization algorithm at present is stochastic gradient descent (SGD; see Recht et al., 2011 for an asynchronous parallellized version of the method). One of the great advantages of SGD is that it can be coded in such a way that the data set can be streamed through a processor, without any need to store it—see Tran, Toulis and Airoldi (2016) for an R implementation for some models in the CRAN package sgd.

It’s worth noting that ScaLE, ZigZag, and BPS can all handle streaming data, producing accurate full-Bayes posterior exploration (i.e., not just MAP estimates) in the $(n \text{ big, } p \text{ small})$ region of problem space. This is in contrast to other methods such as stochastic gradient Langevin dynamics (SGLD, Welling and Teh, 2011), which explores the posterior so slowly that it might as well just be an optimization method. SGLD provides a vivid example of the meta-theorem that if you have a simulation-based method that has an asymptotic convergence proof but that mixes extremely poorly, the convergence proof may be useless as a guide to the practical effectiveness of the method.

- And finally, once again, nobody knows how to make efficient fully Bayesian use of a cluster of GPUs in the $(n, p) = (\text{Big, Big})$ setting, where such
a cluster would be most needed if it could be effectively utilized. If it’s sufficient in your problem to settle for MAP estimates, see Barkalov, Gergel and Lebedev (2016) for one approach to computing them on a GPU cluster.

Three more concluding comments:

• At several points we said things like “if you have access to [hardware configuration X],” but we wish to emphasize that everybody currently has access to the hardware in all four columns of Table 1—including people in academia, not just in industry—by renting this hardware from any of a number of cloud-computing companies, typically for less than US$1 per hour (and universities can often persuade such companies to donate many hours in the cloud to them for free). If you’re currently using only the first column of Table 1 as your hardware resource and you want to begin exploring the Big-Data world, we would encourage you to venture into columns 2 and 3. If you do so, and you can handle the programming (see below), you’ll find, as we have, that for many problems a single GPU is better than 100 CPUs.

• Having just issued an invitation to explore new hardware, it must be admitted that the availability of user-friendly software to make best use of GPUs and CPU clusters is currently nowhere near the level of ease of use of, for example, CRAN packages in R. One promising recent development to note, however, is that at least one hardware manufacturer has recently introduced an external GPU node that makes it possible to drive a GPU with CUDA programs residing on your laptop or desktop—this brings Bayes on GPUs one step further away from the research frontier and closer to day-to-day applications.

• One further note on streaming, GPUs, and the value of contemporary hardware: to work efficiently on a GPU, you either have to (1) hold your data set in the GPU’s memory or (2) stream your data (if it’s too big to fit in memory). Option (2) is how the machine-learning community has obtained its remarkable recent successes with the use of deep learning (e.g., Schmidhuber, 2015) via SGD on a GPU to solve the image classification problem (Krizhevsky, Sutskever and Hinton, 2012).

This brings us to our final meta-theorem: statisticians run the serious risk of being marginalized in the field of data science, ceding the high ground to machine learning when, in our view, this field should involve an equal partnership between mathematical sciences (applied mathematics, statistics), computing sciences (machine learning, database organization and management, the hardware-software interface), and subject-matter expertise in the problem at hand.

We thank Steve for a stimulating paper, and we would be interested in his comments on how sharding methods in general, and his approach in particular, fit into the framework of our table, both currently and in the future.
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