Inference in the Presence of Intractable Normalizing Functions

(Joint work with Jaewoo Park)

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March 2018

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Outline

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Research Areas

- I. Statistical computing
- II. Climate science
- III. Infectious disease modeling
- IV. Spatial models

Lots of overlap

Example: Talk today is on a computing problem motivated by a spatial model for infectious disease

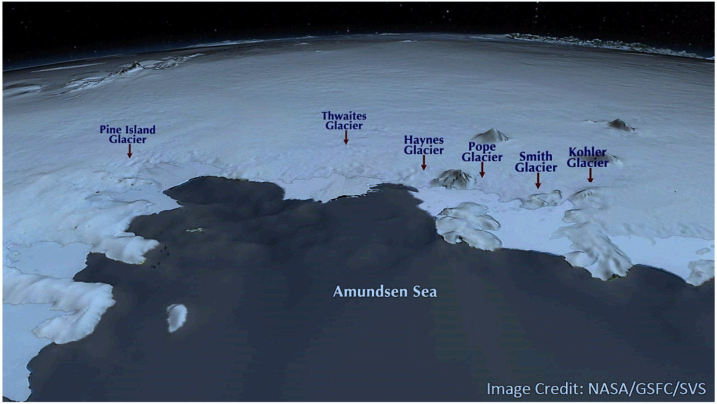
I. Statistical Computing

- Efficient Markov chain Monte Carlo (MCMC) and perfect sampling
- Stopping rules for MCMC algorithms: practical approach with theoretical justification
- Parallelizing MCMC
- Inference for climate and infectious disease models
  - Intractable likelihood functions
  - High-dimensional random effects
- Doubly intractable distributions (today's talk)

II. Climate Science

What is the future of the West Antarctic ice sheet?

(Subject of NC State talk in October 2017)



II. Climate Science: Combining Physics and Data

- Projecting future climate involves sophisticated physical models of climate systems
- Combining physics with observations
- Hierarchical modeling, dimension-reduction approaches, spatial models
- Inference for complex computer models
  - Emulation (approximation) and calibration (parameter inference) for these models using Gaussian processes
  - Challenges
    - high-dimensional spatial observations and model output
    - non-Gaussian spatial data
    - modeling data-model discrepancy

III. Infectious Disease Modeling

UNICEF India (2016)

III. Infectious Disease Research Questions

- Impact of vaccination strategies on infectious diseases
- How do the seasons affect meningitis transmission, and what does this suggest regarding vaccination strategies?
- (New NIH grant) What leads to vaccine refusal? Potential impacts?
- Methods
  - Hierarchical models for dynamics in space and time
  - Susceptible-Infected-Recovered (SIR)-type compartmental models for disease transmission.

Interdisciplinary Setting

- Involves grads, postdoc, faculty from both disciplines
- Cross-disciplinary grant support. Examples:
  - NSF Computational Data-Enabled Science & Engr
  - NSF Sustainable Climate Risk Management
  - Department of Energy (DOE)
  - NIH MIDAS (Models of Infectious Disease Agent Study)
  - Gates Foundation
- Papers published in
  - scientific journals, e.g. *Vaccine, Geoscientific Model Development, Nature Climate Change, Geophysical Research Letters, J of Climate*
  - statistics journals, e.g. *Annals of Applied Stats, JASA, Environmetrics, J of Computational and Graphical Statistics*

IV. Spatial Models

- Efficient methods for high-dimensional non-Gaussian spatial data
  (Subject of NC State talk in November 2017)
  - Latent Gaussian Markov random fields (areal data) and Gaussian process models (continuous-domain spatial data)
- Zero-inflated latent Gaussian hurdle model for modeling spatial data on beetle counts
- Markov attraction-repulsion point process spatial model for respiratory syncitial virus (RSV) infections
- Spatial point process models with dynamics for ant movement data

Outline

Summary

- Doubly intractable distributions pose serious computational challenges
- I will describe a framework for understanding algorithms for such problems
- I will discuss issues and challenges
- I will describe a new algorithm that is computationally expedient for some doubly intractable distributions

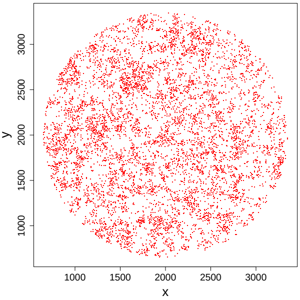
1. Framework, theory, algorithms in Park and Haran (2018) “Bayesian Inference in the Presence of Intractable Normalizing Functions” *Journal of the American Statistical Association*, to appear
2. New algorithm: manuscript in preparation

Models with Intractable Normalizing Functions

- Models with intractable normalizing functions
  - Data: $\mathbf{x} \in \chi$, parameter: $\theta \in \Theta$
  - Model: $h(\mathbf{x}|\theta)/Z(\theta)$, where $Z(\theta) = \int_{\chi} h(\mathbf{x}|\theta)d\mathbf{x}$ is intractable
- Popular examples
  - Social network models: exponential random graph models (Robins et al., 2002; Hunter et al., 2008)
  - Models for lattice data (Besag, 1972, 1974)
  - Spatial point process models: interaction models (Strauss, 1975, Goldstein, Haran et al., 2015)
- Challenge: likelihood-based inference with $Z(\theta)$

Interaction Point Process

- Biologist's interest: study progression of viral infections
- Our goal: use data from imaging of cell cultures to study the spatial structure of an infection
- An *in vitro* cell culture study identifies and locates cells infected with two strains of the human respiratory syncytial virus (RSV-A and RSV-B)



Cells infected with RSV

Question: How does the presence of an infected cell impact infections in neighboring cells?

Attraction-repulsion Model

- Previous models (e.g. Strauss process) did not allow for repulsion *and* attraction
- New point process model (Goldstein, Haran, et al., 2015) allows for both
- Allows us to easily compare interaction behavior for different strains of RSV
- This is a model with an intractable normalizing function
- Existing algorithms take days to run
- This is the motivation for studying existing algorithms and developing new algorithms

Maximum Likelihood (ML) Inference

$$\hat{\theta} = \arg\max_{\theta \in \Theta} h(\mathbf{x}|\theta)/Z(\theta)$$

- Pseudolikelihood approximation (Besag, 1975)
  - Often a poor approximation
  - Awkward in a hierarchical model (it is not compatible with a real probability model)
- Markov chain Monte Carlo Maximum Likelihood (Geyer and Thompson, 1994)
  - Sensitive to choice of importance function
  - Optimization can be unstable
  - For some models, obtaining standard errors is challenging E.g. Our point process model (Goldstein et al., 2015)

Bayesian Inference

- A Bayes approach can sidestep some of the challenges of ML inference.
- Bayesian inference for such models
  - Prior : $p(\theta)$
  - Posterior: $\pi(\theta|\mathbf{x}) \propto p(\theta)h(\mathbf{x}|\theta)/Z(\theta)$
- Inference is generally via Markov chain Monte Carlo (MCMC).
- MCMC is challenging for such models due to $Z(\theta)$.

Markov chain Monte Carlo Basics

- Construct Harris-ergodic Markov chain $\theta_1, \theta_2, \ldots$ with stationary distribution $\pi(\theta \mid \mathbf{x}))$
- Treat $\theta_1, \theta_2, \theta_3, ...$ as if they are samples from $\pi(\theta|\mathbf{x})$
- For any real-valued $g(\cdot)$, approximate $E_\pi(g(\theta))$ by

$$\hat{\mu}_n = \frac{\sum_{i=1}^{n} g(\theta_i)}{n}$$

- Under general conditions, $\hat{\mu}_n \to \mu$ as $n \to \infty$

The Metropolis-Hastings Algorithm

Recipe for constructing Markov chain. Given θ_n, obtain θ_{n+1}

$$\begin{tikzcd}
 & & \boxed{\theta_{n+1} = \theta'} \\
\boxed{\theta_n} \arrow[r] & \boxed{\text{propose } \theta' \sim q(\cdot|\theta_n)} \arrow[ur, "\text{accept}"'] \arrow[dr, "\text{reject}"] & \\
 & & \boxed{\theta_{n+1} = \theta_n}
\end{tikzcd}$$

- Acceptance probability:

$$\alpha = \frac{\pi(\theta'|\mathbf{x})q(\theta_n|\theta')}{\pi(\theta_n|\mathbf{x})q(\theta'|\theta_n)}$$

MCMC with Intractable Normalizing Functions

- Recall:
  - Prior : $p(\theta)$
  - Posterior: $\pi(\theta|\mathbf{x}) \propto p(\theta)h(\mathbf{x}|\theta)/Z(\theta)$
- Acceptance ratio for Metropolis-Hastings algorithm

$$\alpha = \frac{\pi(\theta'|\mathbf{x})q(\theta_n|\theta')}{\pi(\theta_n|\mathbf{x})q(\theta'|\theta_n)} = \frac{p(\theta')Z(\theta_n)h(\mathbf{x}|\theta')q(\theta_n|\theta')}{p(\theta_n)Z(\theta')h(\mathbf{x}|\theta_n)q(\theta'|\theta_n)}$$

Cannot evaluate because of $Z(\theta)$

Outline

Algorithms

Two classes of algorithms for Bayesian inference

I Auxiliary variable methods

- Generate an auxiliary random variate from $f(\theta)$
- Cancel $Z(\theta)$ in the acceptance ratio

II Likelihood approximation methods

- Approximate $Z(\theta)$ using Monte Carlo
- Use approximation, $\hat{Z}(\theta)$ in acceptance ratio

Exchange Algorithm

(Moller et al. (2006); Murray et al. (2007))

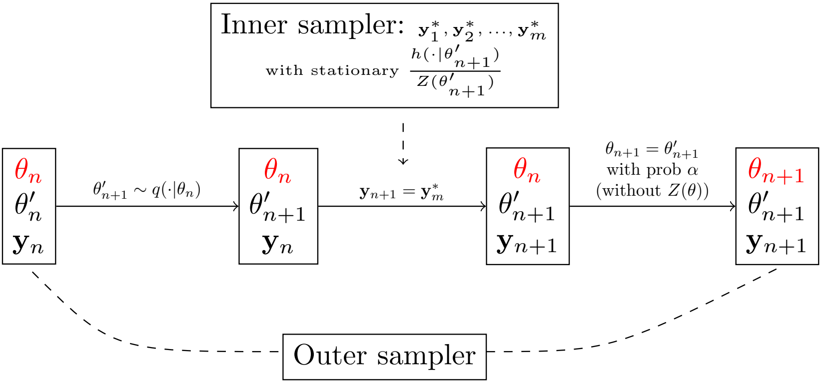
$$\boxed{\begin{matrix}\color{red}{\theta_n}\\ \theta'_n \\ \mathbf{y}_n\end{matrix}} \xrightarrow{\theta'_{n+1} \sim q(\cdot|\theta_n)} \boxed{\begin{matrix}\color{red}{\theta_n}\\ \theta'_{n+1} \\ \mathbf{y}_n\end{matrix}} \xrightarrow{\mathbf{y}_{n+1} \sim \frac{h(\cdot|\theta'_{n+1})}{Z(\theta'_{n+1})} \text{ i.i.d.}} \boxed{\begin{matrix}\color{red}{\theta_n}\\ \theta'_{n+1} \\ \mathbf{y}_{n+1}\end{matrix}} \xrightarrow[\text{with prob } \alpha \text{ (without } Z(\theta))]{\theta_{n+1} = \theta'_{n+1}} \boxed{\begin{matrix}\color{red}{\theta_{n+1}}\\ \theta'_{n+1} \\ \mathbf{y}_{n+1}\end{matrix}}$$

- Goal: obtain next state of Markov chain (θ_{n+1}) from current state (θ_n) by using auxiliary variable **y**
  - Update augmented state ($\theta_n, \theta'_n, \mathbf{y}_n$) instead of updating ($\theta_n$).
  - This cancels out $Z(\theta)$ in acceptance ratio.
  - Then take the marginal samples of (θ_n).

Exchange Algorithm

- Asymptotically exact, that is, $\hat{\mu}_n \to \mu$ as $n \to \infty$
- Very clever and simple (in theory)
- **Requires that we draw exact samples from probability model for each proposed θ**
  - Need to do perfect sampling with Markov chains
  - Infeasible or very expensive in general
- Alternative: Double Metropolis-Hastings (Liang, 2010)

Double Metropolis-Hastings (DMH)



- Theory assumes length of inner and outer sampler go to infinity. **Asymptotically inexact** in practice
- Most practical of algorithms we considered

The Adaptive Exchange Algorithm (AEX)

Liang et al. (2016)

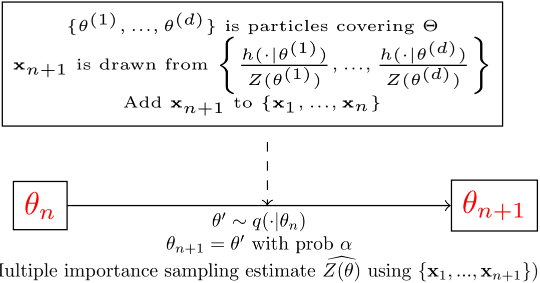
- Basic idea: AEX replaces independent sampling of $\mathbf{y}$ with a re-sampling method.
- With increasing iterations, more samples get added to $\{\mathbf{x}_1, ..., \mathbf{x}_n\}$: re-sampling $\approx$ exact sampling of $\mathbf{y}$ from $h(\mathbf{y}|\theta')/Z(\theta')$.
- Theory: **Asymptotically exact** without perfect sampling
- Slow
- (Extremely) complicated to code/tune
- Huge storage requirements unless sufficient statistics are of low dimensions

Auxiliary Variable Methods: Summary

- Sequential algorithms, not amenable to easy parallelization
- Each iteration involves runnning a (sequential) MCMC algorithm
- Double M-H: asymptotically inexact but easy to code

Likelihood Approximation Method

Atchade, Lartillot and Robert (ALR) Algorithm



- Basic idea: approximate $Z(\theta)$ adaptively through weighted importance sampling. (Atchade et al., 2015)

ALR Algorithm

- With increasing iterations, more samples get added to $\{\mathbf{x}_1, ..., \mathbf{x}_n\}$: approximation $\widehat{Z}_{n+1}(\theta)$ becomes more accurate.
- **Asymptotically exact** without independent sampling
- Memory issues: have to store large number of sampled data used in importance sampling
- Comparable to AEX algorithm in speed
- Outer algorithm is sequential but "inner algorithm" to update importance sampling estimates is amenable to parallelization

Outline

Interaction Point Process Models

θ_1	Mean	95%HPD	ESS	Time(minute)
DMH	1.196	(1.028,1.335)	1343.106	3.935
Gold standard	1.192	(1.031,1.339)	4397.390	

Table: 40,000 MCMC samples

- Simulated low-dimensional point process data $n = 200$. Real problem: $n = 13,000$
  - Data $\mathbf{x} \in R^{200\times 2}$ is coordinates of point process
  - Evaluating $h(\mathbf{x}|\theta)$ requires calculating distance matrix of $\mathbf{x}$.
  - AEX and ALR are impractical (need to store 200×200-dimensional distance matrix with each iteration).
- DMH (**inexact**) is only feasible approach.

Computational Costs

- Computational complexity as a function of data size n
  - Exponential family models: $\mathcal{O}(\mathbf{n})$, point process: $\mathcal{O}(\mathbf{n^2})$
  - Except for fixed costs, complexity of all algorithms are similar
- Memory
  - Without low-dimensional sufficient statistics, huge memory usage in AEX and ALR (**n^2** versus **p**).
  - No memory issues with other algorithms.
- Computational efficiency
  - Likelihood approximation shows better mixing. (high effective sample size).
  - Auxiliary variable approaches are less expensive per iteration. (high effective sample size per second).
  - Hence, roughly speaking, auxiliary variable methods are

Outline

New Emulation-Based Algorithm

- All existing algorithms are computationally very expensive
- An alternative is desirable
- Basic idea:
  - Approximate $Z(\theta)$ using importance sampling on some design points
  - Use Gaussian process emulation approach to interpolate this function at any new value
  - We have some theory to justify this work as number of design points and number of importance sampling draws increases

Computational Benefits

- Can compute in parallel; much of this is done “offline”, before running the algorithm
- Preliminary results: dramatic reduction in computing time.

References

Park and Haran (2018) Bayesian Inference in the Presence of Intractable Normalizing Functions, *Journal of the American Statistical Association*, to appear