The Block-Poisson Estimator for Optimally Tuned Exact Subsampling MCMC

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Overview

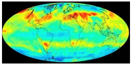
- **Pseudo-Marginal MCMC and Subsampling MCMC**
- **The Block-Poisson likelihood estimator**
- **Optimal subsample size**
- **Empirical results**

Motivation

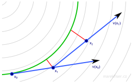
- **MCMC** is still the workhorse for **Bayesian inference**.
- **MCMC is often slooow**
  - Many iterations
  - Need to evaluate the likelihood function in each iteration
- **Hamiltonian Monte Carlo** (**HMC**)
  - quickly traverse high-dimensional parameter spaces
  - ... at the cost of a very large number of gradient evaluations.
- **Subsampling MCMC**: **estimate the likelihood** from a subsample in each MCMC iteration. Fewer evaluations. Faster!

Likelihood evaluations are so expensive nowadays

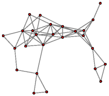
- **High-dimensional spatio-temporal problems** (GMRFs)



- Models where **numerical methods** are needed for evaluating $p(y_i|\theta)$ (ODEs, optimization, etc)



- **Doubly intractable problems** with costly normalization constants (ERGMs)



- So called **Big data** problems with many observations.

The Metropolis-Hastings (MH) algorithm

- Initialize $\theta^{(0)}$ and iterate for $i = 1, 2, ..., N$

  1. Sample $\theta_p \sim q\left(\cdot|\theta^{(i-1)}\right)$ (the **proposal distribution**)

  2. Compute the **acceptance probability**

  $$\alpha = \min\left(1, \frac{p(\mathbf{y}|\theta_p)p(\theta_p)}{p(\mathbf{y}|\theta^{(i-1)})p(\theta^{(i-1)})}\frac{q\left(\theta^{(i-1)}|\theta_p\right)}{q\left(\theta_p|\theta^{(i-1)}\right)}\right)$$

  3. With probability α set $\theta^{(i)} = \theta_p$ and $\theta^{(i)} = \theta^{(i-1)}$ otherwise.

MCMC with an unbiased likelihood estimator

- The likelihood $L(\theta) \equiv p(\mathbf{y}|\theta)$ may be **costly to evaluate**.
- **Unbiased estimator** $\hat{p}(\mathbf{y}|\theta, \mathbf{u})$ of the likelihood

$$\int \hat{p}(\mathbf{y}|\theta, \mathbf{u}) p(\mathbf{u}) d\mathbf{u} = p(\mathbf{y}|\theta)$$

- $\mathbf{u}$ are auxilliary variables used to compute $\hat{p}(\mathbf{y}|\theta, \mathbf{u})$.
- **Monte Carlo integration**: $\mathbf{u}$ are the random numbers. Random effects.
- **Subsampling**: $\mathbf{u}$ are indicators for selected observations.
- Subsampling to estimate the log-likelihood for iid data ($\ell(y_i|\theta) = \log p(y_i|\theta)$)

$$\hat{\ell}(\mathbf{y}|\theta, \mathbf{u}) = \frac{n}{m} \sum_{i \in \mathbf{u}} \ell(y_i|\theta)$$

  where n is the sample size, m the **subsample size**.

The Pseudo-Marginal MH (PMMH) algorithm

- Initialize $\left(\theta^{(0)}, \mathbf{u}^{(0)}\right)$ and iterate for $i = 1, 2, ..., N$

  1. Sample $\theta_p \sim q\left(\cdot|\theta^{(i-1)}\right)$ and $\mathbf{u}_p \sim p(\mathbf{u})$ to obtain the **unbiased** estimate $\hat{p}(\mathbf{y}|\theta_p, \mathbf{u}_p)$
  2. Compute the **acceptance probability**

$$\alpha = \min\left(1, \frac{\hat{p}\left(\mathbf{y}|\theta_p, \mathbf{u}_p\right) p(\theta_p)}{\hat{p}\left(\mathbf{y}|\theta^{(i-1)}, \mathbf{u}^{(i-1)}\right) p(\theta^{(i-1)})} \frac{q\left(\theta^{(i-1)}|\theta_p\right)}{q\left(\theta_p|\theta^{(i-1)}\right)}\right)$$

  3. With probability α set $\left(\theta^{(i)}, \mathbf{u}^{(i)}\right) = \left(\theta_p, \mathbf{u}_p\right)$ and $\left(\theta^{(i)}, u^{(i)}\right) = \left(\theta^{(i-1)}, \mathbf{u}^{(i-1)}\right)$ otherwise.

- Targets a joint distribution $\tilde{p}(\theta, \mathbf{u}|\mathbf{y})$ with marginal $p(\theta|\mathbf{y})$ [1].
- This is true **for any** $\mathbb{V}\left(\hat{p}(\mathbf{y}|\theta, \mathbf{u})\right)$ ...
- ... but $\mathbb{V}\left(\hat{p}(\mathbf{y}|\theta, \mathbf{u})\right)$ has to be low for **efficient sampling**.

Variance reduction - control variates

- Recall: subsampling to estimate the log-likelihood for iid data

$$\hat{\ell}(\mathbf{y}|\theta,\mathbf{u}) = \frac{n}{m}\sum_{i\in\mathbf{u}} \ell(y_i|\theta)$$

- **Difference estimator** with **control variates** $q_i(\theta) \approx \ell(y_i|\theta)$ [2]

$$\hat{\ell}(\mathbf{y}|\theta,\mathbf{u}) = \sum_{i=1}^{n} q_i(\theta) + \frac{n}{m}\sum_{i\in\mathbf{u}} \underbrace{\left(\ell(y_i|\theta) - q_i(\theta)\right)}_{d_i(\theta)}$$

- Two types of control variates
  - **Parameter-expanded** [3]
  - **Data-expanded** [2]
- [2] propose estimating $L(\theta) = \exp\left(\ell(\mathbf{y}|\theta,\mathbf{u})\right)$ by (approximately) **bias-correcting** $\exp\left(\hat{\ell}(\mathbf{y}|\theta,\mathbf{u})\right)$. HMC extension [4].
- Targets a **perturbed posterior** with TV-norm error of $O(n^{-1}m^{-2})$.

Doubly intractable problems

- Doubly intractable

$$p(\theta|\mathbf{y}) \propto \frac{f(\mathbf{y};\theta)p(\theta)}{Z(\theta)}$$

- Common:
  - **Graph-based models (ERGMs)** $Z(\theta)$ is a sum over all graphs
  - **Spatial models** like Potts model.
  - **Directional statistics** $Z(\theta)$ is an intractable integral over the sphere.
- Exponential augmentation trick: $v \sim \mathrm{Exp}(Z(\theta))$

$$\tilde{\pi}(\theta, v) \propto \exp\left(-vZ(\theta)\right) f(\mathbf{y};\theta)p(\theta)$$

Variance reduction - dependent PMMH

- What really matters for MH is the variance of

$$\log \frac{\hat{p}\left(\mathbf{y}|\theta_p, \mathbf{u}_p\right)}{\hat{p}\left(\mathbf{y}|\theta^{(i-1)}, \mathbf{u}^{(i-1)}\right)}$$

- **Correlated Pseudo Marginal** (**CPM**) [5, 6]: correlate the $\mathbf{u}$ over MH iterations using an autoregressive proposal $\mathbf{u}^{(i)} = \phi\mathbf{u}^{(i-1)} + \epsilon$.

- **Subsampling** context: correlate binary subsampling indicators with Gaussian copula [2].

- **Block Pseudo Marginal** (**BPM**) [7]: partition $\mathbf{u} = (u_1, ..., u_m)$ in blocks and **update a single block** jointly with θ at each iteration.

The Block-Poisson estimator

- The **Block-Poisson estimator** of the likelihood $L(\theta)$:

$$\hat{L}_B(\theta) \equiv \exp(q) \prod_{l=1}^{\lambda} \xi_l$$

$$\xi_l \equiv \exp\left(\frac{a+\lambda}{\lambda}\right) \prod_{h=1}^{\mathcal{X}_l} \left(\frac{\hat{d}_m^{(h,l)} - a}{\lambda}\right)$$

  - $q \equiv \sum_{i=1}^{n} q_i(\theta)$ is the sum of the control variates
  - $\lambda \in \mathbb{N}^+$ and $a \in \mathbb{R}$
  - $\hat{d}_m^{(h,l)}$ is an unbiased estimator of $d = \ell - q$ from a batch of m obs
  - $\mathcal{X}_1, ..., \mathcal{X}_\lambda \overset{iid}{\sim} \text{Pois}(1)$
- Product form allows us to use **Block Pseudo Marginal** (**BPM**).
- $\hat{L}_B(\theta)$ requires on average λm evaluations of ℓ_i's.

Properties of the Block-Poisson estimator

$$\hat{L}_B(\theta) = \exp(q) \prod_{l=1}^{\lambda} \xi_l, \text{ where } \xi_l = \exp\left(\frac{a+\lambda}{\lambda}\right) \prod_{h=1}^{\mathcal{X}_l} \left(\frac{\hat{d}_m^{(h,l)} - a}{\lambda}\right)$$

- **Unbiased**: $\mathbb{E}\left(\hat{L}_B(\theta)\right) = L(\theta)$ for all $\theta \in \Theta$.
- **Positive**: $\hat{L}_B(\theta)$ is almost surely positive only if $\hat{d}_m^{(h,l)} \geq a$ almost surely for all h and l.
- For a given λ, $\mathbb{V}\left(\hat{L}_B(\theta)\right)$ is minimized for $a = d - \lambda$.
- $\mathbb{V}\left(\hat{L}_B(\theta)\right) = \mathbb{V}\left(\hat{L}_P(\theta)\right)$ where $\hat{L}_P(\theta)$ is the usual Poisson estimator in e.g. [8].

Signed PMMH

- Forcing a to be a **lower bound** for all $\hat{d}_m^{(h,l)}$ is impractical:
  - Usually need to know ℓ_i for all data points.
  - $a = d - \lambda$ implies that λ will be large. Costly!

- **Soft lower bound:** $\Pr(\hat{d}_m^{(h,l)} \geq a)$ close to one. More efficient, but $\hat{L}_B(\theta) < 0$ possible.

- **Signed PMMH** [9]
  - **Run PMMH on absolute value** $\left|\hat{L}_B(\theta)\right| p(\theta)$
  - **Correct for the sign** $s = \operatorname{Sign}\left(\hat{L}_B(\theta)\right)$ using importance sampling

$$\widehat{\mathbb{E}\psi(\theta)} = \frac{\sum_{i=1}^N \psi(\theta^{(i)}) s^{(i)}}{\sum_{i=1}^N s^{(i)}}.$$

Optimal tuning of Signed PMMH based on $\hat{L}_B(\theta)$

- **Optimal** subsample size m in regular PMMH?
- Minimize (normalized) asymptotic variance of PMMH estimates of $\mathbb{E}\left[\psi(\theta)\right]$ per unit of computing time

$$\mathrm{CT}(m) \propto m \cdot \mathrm{IF}(\sigma^2_{\log \hat{L}})$$

- Regular PMMH is optimal when $\mathbb{V}(\log \hat{L}(\theta)) \approx 1$ [10, 11].
- **Optimal** λ and m in **signed PMMH** minimizes

$$\mathrm{CT}(\lambda, m) \propto m\lambda \cdot \frac{\mathrm{IF}\left[\sigma^2_{\log|\hat{L}_B|}(\lambda, m)\right]}{\left(2\tau(\lambda, m) - 1\right)^2}$$

- Optimal λ and m balances
  1. The **cost** of computing $\hat{L}_B$, which is $m\lambda$ on average
  2. **MH inefficiency**, IF
  3. Probability of a **positive sign** $\tau(\lambda, m)$

Optimal tuning of Signed PMMH

- To compute $\mathrm{CT}(\lambda, m)$, we need expressions for:
  - $\mathrm{IF}(\cdot)$
  - $\sigma^2_{\log|\hat{L}_B|}(\lambda, m)$
  - $\tau(\lambda, m)$

- The **derivation of** IF is an extension of the theory in [10] to blocked signed PMMH.

- Idealized assumptions:
  - Perfect MH proposal for θ
  - $\sigma^2_{\log|\hat{L}_B|}$ is not a function of θ

- **Heuristic guidelines**. But accurate in experiments.

- **Conservative guidelines**: $m\lambda$ is not suggested too small.

$\tau \equiv \Pr(\hat{L}_B \geq 0)$

- Under the minimum variance condition $a = d - \lambda$

$$\hat{L}_B(\theta) = \exp(q) \prod_{l=1}^{\lambda} \xi_l, \text{ where } \xi_l = \exp\left(\frac{d}{\lambda}\right) \prod_{h=1}^{\mathcal{X}_l} \left(\frac{\hat{d}_m^{(h,l)} - d}{\lambda} + 1\right)$$

- $\hat{L}_B(\theta) > 0$ whenever an even number of ξ_l are negative.
- $\xi_l > 0$ whenever an even number of $A_m = \frac{\hat{d}_m - d}{\lambda} + 1$ are negative.
- Applying a result from Feller's first book twice:

$$\Pr(\hat{L}_B \geq 0) = \frac{1}{2}\left[1 + (1 - 2\Psi(m, \lambda))^{\lambda}\right]$$

where

$$\Psi(m, \lambda) \equiv \Pr(\xi_l < 0) = \frac{1}{2} \sum_{j=1}^{\infty} \left[1 - (1 - 2\Pr(A_m < 0))^{j}\right] \Pr(\mathcal{X}_l = j),$$

$\mathcal{X}_l \overset{iid}{\sim} \text{Pois}(1)$ and $A_m = \frac{\hat{d}_m - d}{\lambda} + 1$.

$\sigma^2_{\log\left|\hat{L}_B\right|}(\lambda, m)$

- Under the condition $a = d - \lambda$ we have

$$\begin{aligned}\log\left|\hat{L}\right| &= q + d + \sum_{l=1}^{\lambda}\sum_{h=1}^{\mathcal{X}_l} \log\left(\left|\frac{\hat{d}_m^{(h,l)} - d}{\lambda} + 1\right|\right) \\ &= q + d + \frac{1}{2}\sum_{l=1}^{\lambda}\sum_{h=1}^{\mathcal{X}_l} \log\left(\frac{\hat{d}_m^{(h,l)} - d}{\lambda} + 1\right)^2\end{aligned}$$

- $\hat{d}_m^{(h,l)} \sim \text{Normal} \Rightarrow \sigma^2_{\log\left|\hat{L}_B\right|}(\lambda, m)$ is the variance of a random sum of logs of non-central χ^2 variables.
- Non-central χ^2 is a Poisson mixture of central χ^2 [12]
- Moments of log central χ^2 are known from [13]
- Law of total variance

Optimal tuning - normal case

- Assume $\hat{d}_m^{(h,l)} \sim$ Normal.
- Both $\Pr(\hat{L}_B \geq 0)$ and $\sigma^2_{\log|\hat{L}_B|}(\lambda, m)$ are functions of the variance of $\hat{d}_m^{(h,l)}$

$$\mathbb{V}(\hat{d}_m^{(h,l)}(\theta)) = \frac{n^2}{m}\sigma^2_{d_i}(\theta)$$

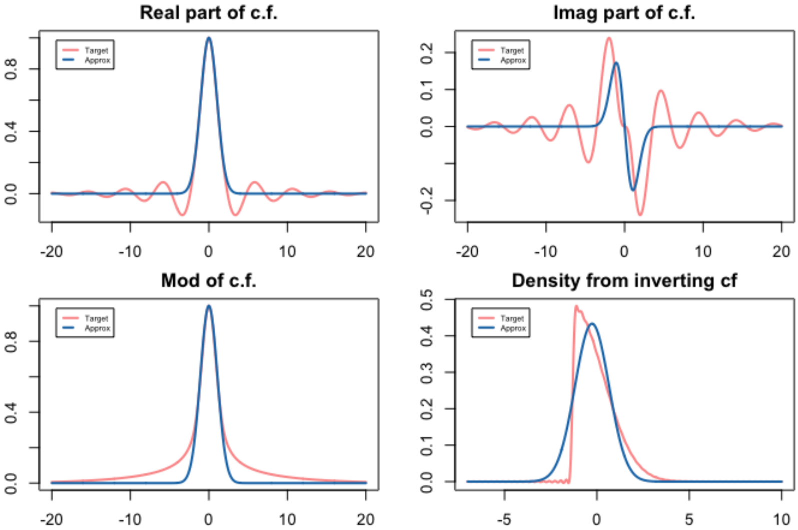
- Optimal tuning therefore depends on $\sigma^2_{d_i}(\theta)$.
- Solution: estimate $\sigma^2_{d_i}(\theta)$ from a subsample for some selected θ.
- What if $\hat{d}_m^{(h,l)}$ are not normal?
- Set $m = 20$ and rely on the CLT. Optimize only λ.
- However, numerical experiments tell us that $m = 1$ is optimal.

Optimal tuning - mixture of normals case

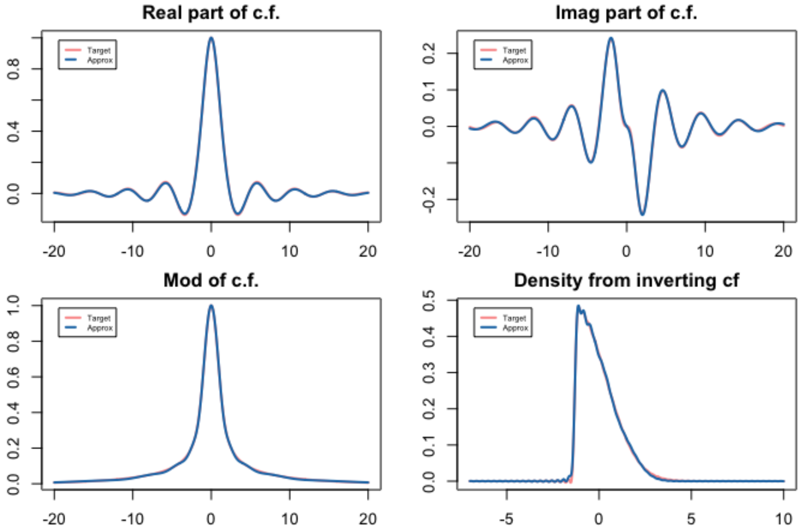
- We can instead assume that $\hat{d}_m^{(h,l)}$ follows a **mixture of normals.**
- Mixture of normals are **universal approximators**.
- Both $\Pr(\hat{L}_B \geq 0)$ and $\sigma^2_{\log|\hat{L}_B|}$ are still **tractable**.
- ... but estimating $\sigma^2_{d_i}(\theta)$ is not enough anymore.
- How to fit a mixture of normals to $\hat{d}_m^{(h,l)}$?

- **Matching characteristic functions** (c.f.)
  1. Fit any distribution to a subsample of d_i's and get the c.f. $\varphi_d(t)$.
  2. Compute the c.f. of $\hat{d}_m^{(h,l)}$ as $\varphi_{\hat{d}_m}(t) = (\varphi_d(t/m))^m$.
  3. Approximate the distribution of $\hat{d}_m^{(h,l)}$ by a normal mixture by L2-matching of c.f.'s. Plancherel's theorem.

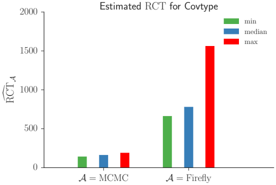
Matching a 1-component MoN to skewed normal



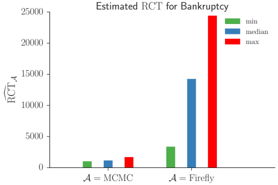
Matching a 5-component MoN to skewed normal



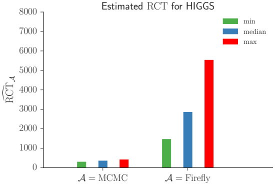
Relative CT - logistic regression on three real datasets



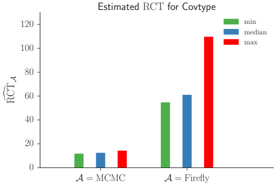
(A) Covtype data.



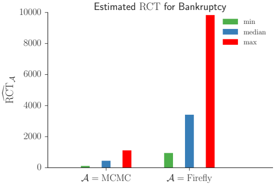
(B) Bankruptcy data.



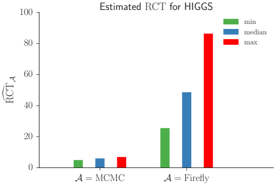
(C) HIGGS data.



(A) Covtype data.



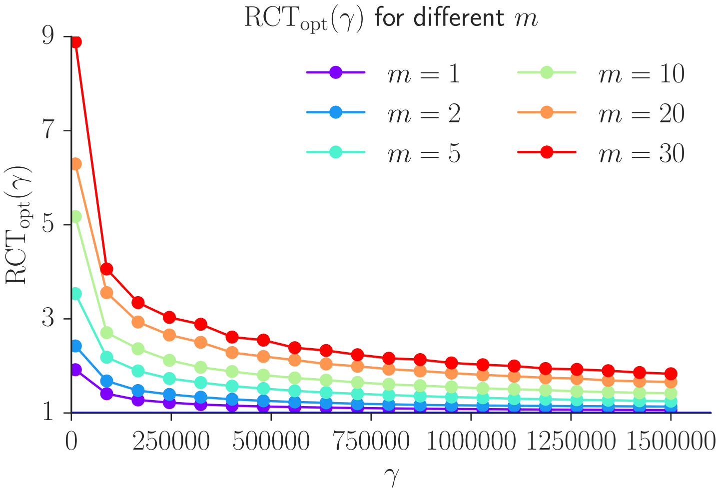
(B) Bankruptcy data.



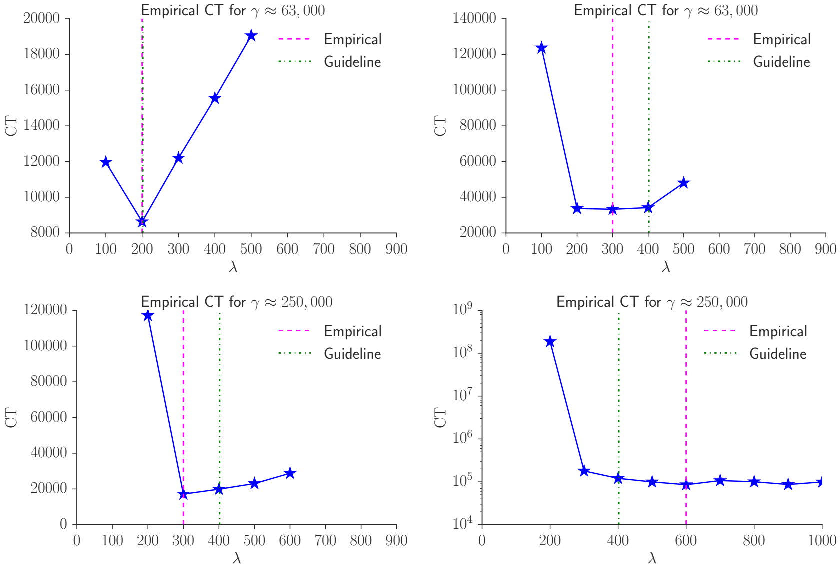
(C) HIGGS data.

Relative CT: Signed PMMH vs Approximate PMMH

- $\gamma = n^2\sigma_{d_i}^2$



Checking the optimality guidelines



(A) γ does not depend on θ.

(B) γ depends on θ.

Conclusions

- **Subsampling** to speed up MCMC and HMC.
- **Control variates** and **slowly evolving subsamples** are important for efficiency.
- **Block-Poisson** is an **unbiased** and **efficient** estimator of the likelihood.
- **Optimal tuning of Signed PMMH** with Block-Poisson estimator.
- **Very large speed-ups** compared to regular MCMC and FireFly MC.
- Can be used to optimally tune Signed PMMH in **doubly intractable problems**.

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