Hierarchical Monte Carlo Fusion Ryan Chan

Murray Pollock (Newcastle), Adam Johansen (Warwick), Gareth Roberts (Warwick)

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The Alan Turing Institute

Outline

Monte Carlo Fusion Fork-and-join Constructing a rejection sampler Double Langevin Approach

Hierarchical Fusion Time-adapting Monte Carlo Fusion Divide-and-Conquer SMC with Fusion

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Logistic Regression Example

Ongoing directions

- Monte Carlo Fusion

Fork-and-join

Fusion Problem

• Target:

$$\pi(\boldsymbol{x}) \propto \prod_{c=1}^{C} f_c(\boldsymbol{x})$$

where each *sub-posterior*, $f_c(\mathbf{x})$, is a density representing one of the *C* distributed inferences we wish to unify

• Assume we can sample $\mathbf{x}^{(c)} \sim f_c(\mathbf{x})$

• Applications:

- Expert elicitation: combining views of multiple experts
- Privacy setting
- Big Data (by construction)
- Tempering (by construction)

Fork-and-join

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Fusion for Big Data

- Consider we have data x with a large number of observations n
- The likelihood $\ell(\mathbf{x} \mid \theta)$ becomes expensive to calculate
 - This makes MCMC prohibitively slow for big data
- Potential solution:

$$\pi(\theta \mid \mathbf{x}) \propto \prod_{i=1}^{n} \ell(\mathbf{x} \mid \theta) \pi(\theta) = \prod_{c=1}^{C} \ell(\mathbf{x}_{c} \mid \theta) \pi(\theta)^{\frac{1}{C}}$$

where \mathbf{x}_c denotes the *c*-th subset for c = 1, ..., C and $\pi(\theta) = \prod_{c=1}^{C} \pi(\theta)^{\frac{1}{c}}$ is the prior

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Fork-and-join

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- Consider the *power-tempered target distribution π*_β(**x**) = [π(**x**)]^β for β ∈ (0, 1]
- MCMC can become computationally expensive to sample from multi-modal densities and can get stuck in modes
- Potential solution:

$$\pi(\mathbf{x}) = \pi(\mathbf{x})^{rac{1}{eta} \cdot eta} = \prod_{c=1}^{rac{1}{eta}} \pi_{eta}(\mathbf{x})$$

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Fork-and-join

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The fork-and-join approach:



Fork-and-join

Current Fork-and-Join Methods

- Several fork-and-join methods have been developed. For instance
 - Kernel density averaging [Neiswanger et al., 2013]
 - Weierstrass sampler [Wang and Dunson, 2013]
 - Consensus Monte Carlo [Scott et al., 2016]
- A primary weakness of these methods is that the recombination is inexact in general and involve approximations
- However, Monte Carlo Fusion [Dai et al., 2019] is exact

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Constructing a rejection sampler

Constructing a rejection sampler - An Extended Target

Proposition

Suppose that $p_c(\mathbf{y} | \mathbf{x}^{(c)})$ is the transition density of a stochastic process with stationary distribution $f_c^2(\mathbf{x})$. The (C+1)d-dimensional (fusion) density proportional to the integrable function

$$g(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(C)},\boldsymbol{y}) \propto \prod_{c=1}^{C} \left[f_c^2(\boldsymbol{x}^{(c)}) p_c(\boldsymbol{y} \mid \boldsymbol{x}^{(c)}) \cdot \frac{1}{f_c(\boldsymbol{y})} \right]$$

admits the marginal density π for \mathbf{y} .

• Main idea: If we can sample from g, then we can can obtain a draw from the fusion density $(\mathbf{y} \sim \pi)$

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admits the marginal density π for **y**.

Main idea: If we can sample from g, then we can can obtain a draw from the fusion density (y ~ π)

Constructing a rejection sampler

Rejection Sampling (Double Langevin Approach)

- There are many possible choices for $p_c(\mathbf{y} \mid \mathbf{x})$
- Let p_c(y | x) := p_{T,c}(y | x), the transition density of the d-dimensional (double) Langevin (DL) diffusion processes X_t^(c) for c = 1,..., C, from x to y for a pre-defined time T > 0 given by

 $\mathrm{d}\boldsymbol{X}_t^{(c)} = \nabla \log f_c(\boldsymbol{X}_t^{(c)}) \mathrm{d}t + \mathrm{d}\boldsymbol{W}_t^c,$

- $W_t^{(c)}$ is *d*-dimensional Brownian motion
- abla is the gradient operator over $oldsymbol{x}$
- Has stationary distribution $f_c^2(\mathbf{x})$

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$$h(\mathbf{x}^{(1)},\ldots,\mathbf{x}^{(C)},\mathbf{y}) \propto \prod_{c=1}^{C} \left[f_c(\mathbf{x}^{(c)}) \right] \cdot \exp\left(-\frac{C \cdot \|\mathbf{y} - \bar{\mathbf{x}}\|^2}{2T}\right)$$

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•
$$\bar{x} = \frac{1}{C} \sum_{c=1}^{C} x^{(c)}$$

• T is an arbitrary positive constant

Constructing a rejection sampler

Rejection Sampling (Double Langevin Approach)

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- Monte Carlo Fusion

Constructing a rejection sampler

Rejection Sampling - acceptance probability

• Acceptance probability:

$$\frac{g(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(C)},\boldsymbol{y})}{h(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(C)},\boldsymbol{y})} \propto \rho \cdot Q$$

where

$$\begin{cases} \rho \coloneqq e^{-\frac{C\sigma^2}{2T}}, & \sigma^2 = \frac{1}{C} \sum_{c=1}^C \left\| \boldsymbol{x}^{(c)} - \bar{\boldsymbol{x}} \right\|^2 \\ Q \coloneqq \mathbb{E}_{\bar{\mathbb{W}}} \left(\prod_{c=1}^C \left[\exp\left\{ -\int_0^T \left(\phi_c(\boldsymbol{x}_t^{(c)}) - \Phi_c \right) \mathrm{d}t \right\} \right] \right) \end{cases}$$

where $\overline{\mathbb{W}}$ denotes the law of *C* independent Brownian bridges $\mathbf{x}_t^{(1)}, \ldots, \mathbf{x}_t^{(C)}$ with $\mathbf{x}_0 = \mathbf{x}^{(c)}$ and $\mathbf{x}_T^{(c)} = \mathbf{y}$

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Q Acceptance Probability

$$Q \coloneqq \mathbb{E}_{\bar{\mathbb{W}}} \Big(\prod_{c=1}^{C} \Big[\exp \Big\{ - \int_{0}^{T} \Big(\phi_{c}(\mathbf{x}_{t}^{(c)}) - \Phi_{c} \Big) \mathrm{d}t \Big\} \Big] \Big)$$

where

•
$$\phi_c(\mathbf{x}) = \frac{1}{2} \left(\|\nabla \log f_c(\mathbf{x})\|^2 + \Delta \log f_c(\mathbf{x}) \right)$$

- Φ_c are constants such that for all \boldsymbol{x} , $\phi_c(\boldsymbol{x}) \ge \Phi_c$ for $c \in \{1, \dots, C\}$
- Events of probability Q can be simulated using Poisson thinning and methodology called Path-space Rejection Sampling (PSRS) or the Exact Algorithm (Beskos et al. [2005], Beskos et al. [2006], Pollock et al. [2016])

Constructing a rejection sampler

Interpretation

 Correct a simple average x̄ of sub-posterior values to a Monte Carlo draw from π(x) with acceptance probability ρ · Q



Double Langevin Approach

Double Langevin Approach - Summary

• Proposal:

$$h(\mathbf{x}^{(1)},\ldots,\mathbf{x}^{(C)},\mathbf{y}) \propto \prod_{c=1}^{C} \left[f_c(\mathbf{x}^{(c)}) \right] \cdot \exp\left(-\frac{C \cdot \|\mathbf{y}-\bar{\mathbf{x}}\|^2}{2T}\right)$$

• Accept y as a draw from fusion density π with probability:

$$\frac{g(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(C)},\boldsymbol{y})}{h(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(C)},\boldsymbol{y})} \propto \rho \cdot Q$$

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• Monte Carlo Fusion Algorithm:

- 1. Simulate $m{x}^{(c)} \sim f_c(m{x})$ and $m{y} \sim \mathcal{N}(m{ar{x}}, rac{T\mathbb{I}_d}{C})$
- 2. Accept **y** with probability $\rho \cdot Q$

Double Langevin Approach

Double Langevin Approach - Summary

• Proposal:

$$h(\mathbf{x}^{(1)},\ldots,\mathbf{x}^{(C)},\mathbf{y}) \propto \prod_{c=1}^{C} \left[f_c(\mathbf{x}^{(c)}) \right] \cdot \exp\left(-\frac{C \cdot \|\mathbf{y}-\bar{\mathbf{x}}\|^2}{2T}\right)$$

• Accept \boldsymbol{y} as a draw from fusion density π with probability:

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-Hierarchical Fusion

Limitations of above rejection sampler

- 1. Scalability: the acceptance probability of Monte Carlo fusion can be small, especially when *C* is large or *d* is large
- 2. Use of simple average \bar{x} of sub-posterior samples as the proposal
 - but should we use a weighted average?
- 3. Use of same time T for each sub-posterior
 - but different cores / sub-posteriors could contain different amounts of information
- 4. **PSRS**: methodology for PSRS can be computationally expensive

Aim: To construct a fusion algorithm / framework to alleviate some of these limitations
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Hierarchical Monte Carlo Fusion

1. Scalability with C

The Monte Carlo Fusion algorithm implies a fork-and-join approach:



Hierarchical Monte Carlo Fusion

Solution: Hierarchical Monte Carlo Fusion

- We could perform fusion in a proper divide-and-conquer framework
- Two possible choices are hierarchical (left) and progressive (right) trees



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Hierarchical Monte Carlo Fusion

Hierarchical Fusion

Example

• Target:
$$\pi(x) \propto e^{-\frac{x^4}{2}}$$

• Sub-posteriors:
$$f_c(x) = e^{-\frac{x^4}{2C}}$$
 for $c = 1, \dots, C$



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Hierarchical Monte Carlo Fusion

Hierarchical Fusion

Time-adapting Monte Carlo Fusion

Time-adapting Monte Carlo Fusion

2. Use of simple average \bar{x} of sub-posterior samples as the proposal

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• We assign weights to each sub-posterior and use a weighted

• Time T is adapted for each posterior: $T_c = \frac{T}{w}$ for



Time-adapting Monte Carlo Fusion

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• Solution: Time-adapting Monte Carlo Fusion

• We assign weights to each sub-posterior and use a weighted average: $\tilde{x} = \sum_{c} w_{c} x^{(c)} / \sum_{c} w_{c}$

• Time T is adapted for each posterior: $T_c = \frac{T}{w_c}$ for $c = 1, \dots, C$





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Time-adapting Monte Carlo Fusion

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- Time-adapting Monte Carlo Fusion Algorithm:
 - 1. Choose time T and weights for sub-posteriors $w_c, c = 1, ..., C$
 - 2. Simulate $\mathbf{x}^{c} \approx I_c(\mathbf{x})$ and $\mathbf{y} \approx \mathcal{N}(\mathbf{x}, \sum_{c} V_{c})$
 - 3. Accept **y** with probability $\rho^{ta} \cdot Q^{ta}$



Time-adapting Monte Carlo Fusion

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• Time-adapting Monte Carlo Fusion Algorithm:

- 1. Choose time T and weights for sub-posteriors $w_c, c = 1, \ldots, C$
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Divide-and-Conquer SMC

4. PSRS: methodology for PSRS can be computationally expensive

- Solution: Sequential Monte Carlo in the hierarchical fusion framework
- Rejection sampling can be wasteful: large number of proposed samples are rejected
- Motives the use of Sequential Importance Sampling / Resampling ideas
 - Replace the rejection sampling steps with importance sampling steps
 - Fits into the Divide-and-Conquer SMC (D&C-SMC) framework by Lindsten et al. [2017]

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Logistic Regression Example - Taiwan default payments

• Predicting if customers defaulted on their payments using gender and education levels (n = 30,000 and d = 5)

• Split into C = 32 subsets and apply the following methods:

- 1. Consensus Monte Carlo [Scott et al., 2016]
- 2. Kernel density averaging [Neiswanger et al., 2013]
- 3. Weierstrass rejection sampler [Wang and Dunson, 2013]
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5. Hierarchical Time-adapting SMC Fusion

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5. Hierarchical Time-adapting SMC Fusion

Logistic Regression Example - Taiwan default payments

- Choose a time T = 0.5
- Use balanced hierarchical tree where we combine m = 2sub-posteriors at each level, i.e. have L = 6 levels in the tree
- Weights are chosen according to how much data they have relative to the bottom level:
 - At L = 6: sub-posteriors are given weight $w_c = 1$ for c = 1, ..., 32, i.e. $T_c = 0.5$
 - At L = 5: sub-posteriors are given weight $w_c = 2$ for c = 1, ..., 16 (have twice more data than the start), i.e. $T_c = \frac{0.5}{2} = 0.25$
 - and so on up the levels...

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How to apply Hierarchical Time-adapting SMC Fusion

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• To compare methods we calculate the integrated absolute distance

$$IAD = \frac{1}{2d} \sum_{j=1}^{d} \int \left| \hat{f}(\mathbf{x}_{j}) - f(\mathbf{x}_{j}) \right| dx_{j}$$

where $\hat{f}(\mathbf{x}_j)$ is the marginal density for \mathbf{x}_j based on the method applied and $f(\mathbf{x}_j)$ is the benchmark estimate (obtained using NUTS with Stan)

• Fix computational cost by restricting run-time allowed for algorithm

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- Logistic Regression Example

Logistic Regression Example - Taiwan default payments



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Ongoing directions

Combining conflicting sub-posteriors

- Confidential fusion (Con-fusion): where sharing information/data between cores is not permitted
- Bayesian Fusion: tailored to big data Bayesian problems
- Different proposals: e.g. Ornstein-Uhlenbeck bridges, more general Langevin diffusion with pre-conditioning matrix for each sub-posterior

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• Theory for D&C-SMC with Monte Carlo Fusion

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